# STIC Search Report
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STIC Database Tracking Number: 171184

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| **TO: Deborah Lambkin**<br>**Location: REM-5B09/5C18**<br>**Art Unit: 1626**<br>**November 22, 2005**<br><br>**Case Serial Number: 10/678331** | **From: P. Sheppard**<br>**Location: Remsen Building**<br>**Phone: (571) 272-2529**<br><br>**sheppard@uspto.gov** |

## Search Notes

171184

Access DB# _____

# SEARCH REQUEST FORM

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**Scientific and Technical Information Center**

Requester's Full Name: Deborah Kemblem Examiner # : 71300 Date: 11/9/07
Art Unit: 1626 Phone Number 30-2-0698 Serial Number: 10/678,331
Mail Box and Bldg/Room Location: Rem 5309 Results Format Preferred (circle): PAPER DISK E-MAIL

**If more than one search is submitted, please prioritize searches in order of need.**

**********

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

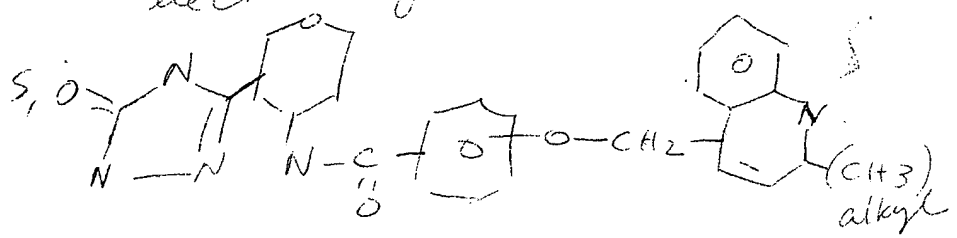
Title of Invention: TRIAZOLONE & TRIAZOLETHION . . .

Inventors (please provide full names): B. W. King

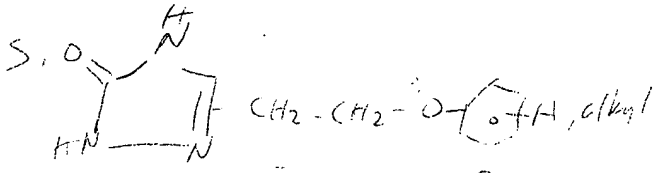
Earliest Priority Filing Date: _____

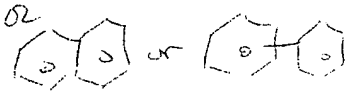
***For Sequence Searches Only*** *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

elected species




surrogate compound




Compd looks too large to search, but would like to try it if ok. Thanks

**********

| STAFF USE ONLY | Type of Search | Vendors and cost where applicable |
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| Searcher Phone #: _____ | AA Sequence (#)_____ | Dialog _____ |
| Searcher Location: _____ | Structure (#) _____ | Questel/Orbit _____ |
| Date Searcher Picked Up: _____ | Bibliographic _____ | Dr.Link _____ |
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PTO-1590 (8-01)

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     FILE HCAPLUS

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     DICTIONARY FILE UPDATES:  21 NOV 2005  HIGHEST RN 868586-21-4

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*                                                                    *
* The CA roles and document type information have been removed from  *
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

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 substance identification.

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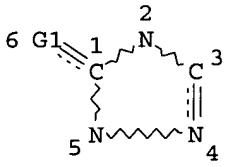


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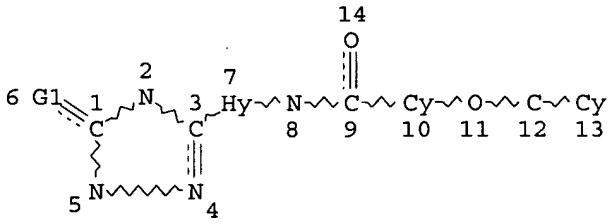

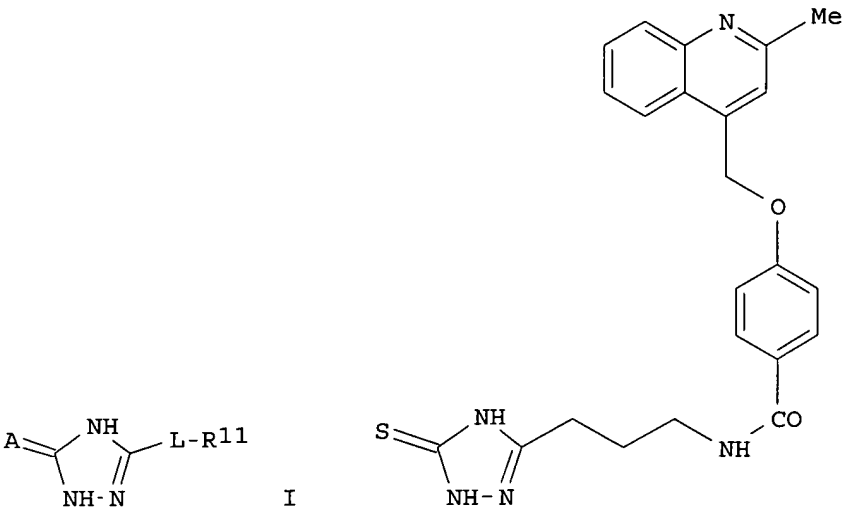

I II

AB The present application describes novel hydantoin derivs. (shown as I; A = O, S; L-R11 represents a very large variety of substituents and is defined in the claims; e.g. II) or pharmaceutically acceptable salt or prodrug forms thereof, which are useful as inhibitors of matrix metalloproteinases (MMP), TNF-α converting enzyme (TACE), aggrecanase, or a combination thereof. Some examples of I exhibit Ki's <10 μM but individual data are not presented. Although the methods of preparation are not claimed, 37 example prepns. are included. For example, II was prepared in 4 steps (100, 66, 73 and 82%, resp.) starting with condensation of Et 4-aminobutyrate hydrochloride with 4-(2-methylquinolin-4-ylmethoxy)benzoyl chloride hydrochloride followed by base hydrolysis to the acid, followed by hydrazide formation with thiosemicarbazide followed by cyclization.

IT **681284-32-2P 681284-35-5P 681284-36-6P**
**681284-41-3P 681284-46-8P 681284-50-4P**
**681284-62-8P 681284-63-9P 681284-67-3P**
**681284-68-4P 681284-70-8P 681284-71-9P**
**681284-80-0P 681284-81-1P 681284-91-3P**
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**681285-46-1P 681285-47-2P 681285-51-8P**
**681285-52-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of triazolone and triazolethione inhibitors of matrix metalloproteinases and/or TNF-α converting enzyme as anti-inflammatory agents)

RN 681284-32-2 HCAPLUS

CN Benzamide, N-[(3S,4R)-3-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)tetrahydro-2H-pyran-4-yl]-4-[(2-methyl-4-quinolinyl)methoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

yl)tetrahydro-2H-pyran-4-yl]-4-[(2-methyl-4-quinolinyl)methoxy]-, rel-, trifluoroacetate (9CI) (CA INDEX NAME)

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CRN 681284-35-5
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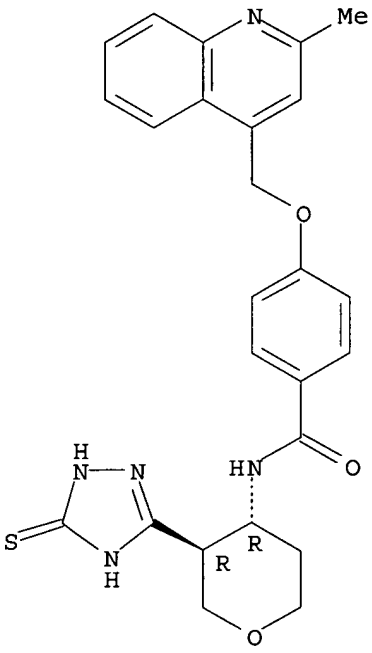
Relative stereochemistry.



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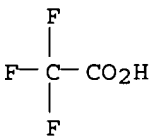

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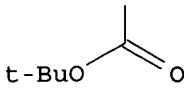
Absolute stereochemistry.

PAGE 2-A

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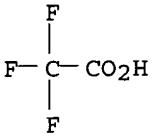


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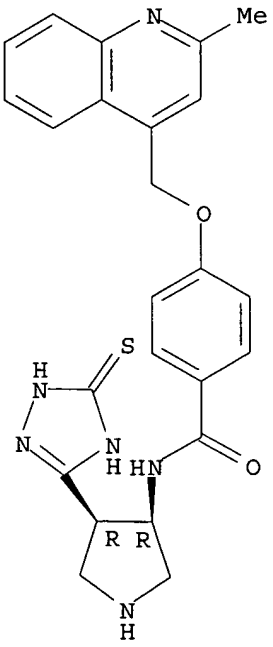
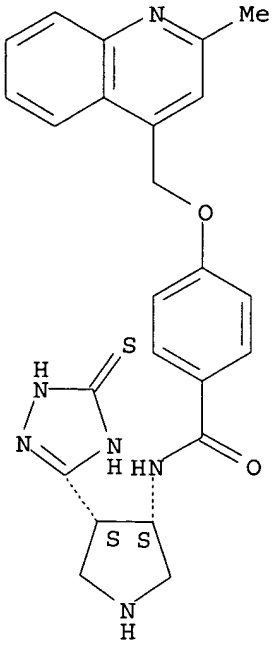
CRN 681284-49-1
CMF C24 H24 N6 O2 S

Relative stereochemistry.





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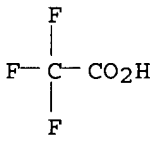
CRN 76-05-1
CMF C2 H F3 O2



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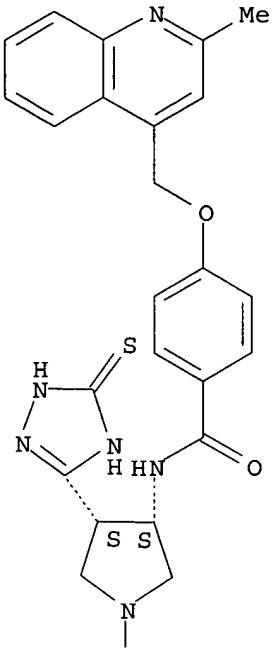
CN Benzamide, N-[(3S,4S)-1-acetyl-4-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3-pyrrolidinyl]-4-[(2-methyl-4-quinolinyl)methoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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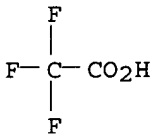
CM 2

CRN 76-05-1
CMF C2 H F3 O2



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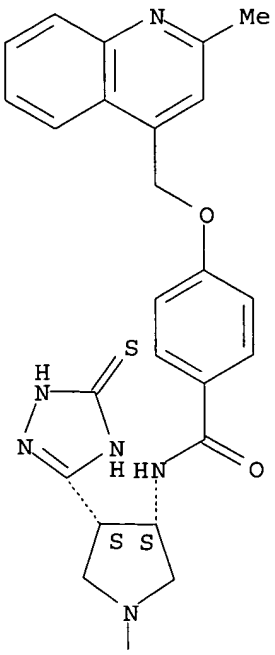
CN Benzamide, N-[(3S,4S)-4-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-1-propyl-3-pyrrolidinyl]-4-[(2-methyl-4-quinolinyl)methoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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Pr-n

CM 2

CRN 76-05-1
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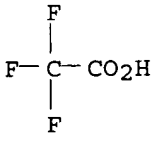

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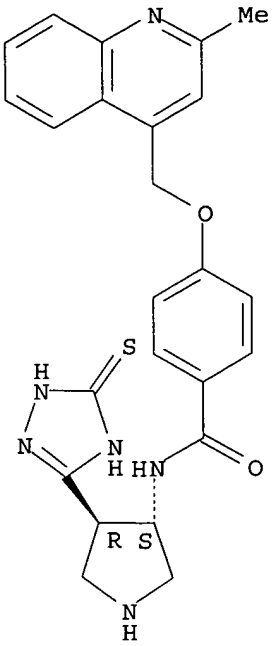
Relative stereochemistry.



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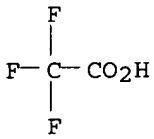
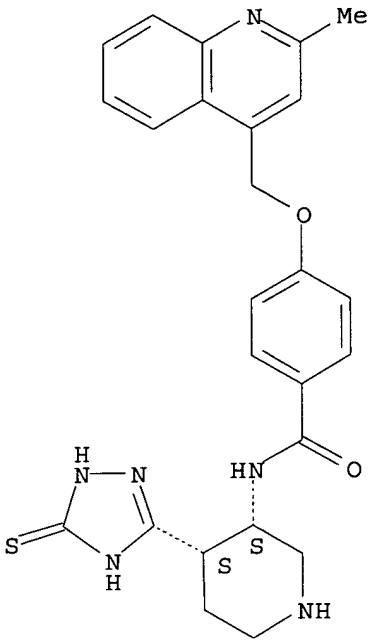


RN 681284-91-3 HCAPLUS
CN 1-Piperidinecarboxylic acid, 4-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3-[[4-[(2-methyl-4-quinolinyl)methoxy]benzoyl]amino]-, 1,1-dimethylethyl ester, (3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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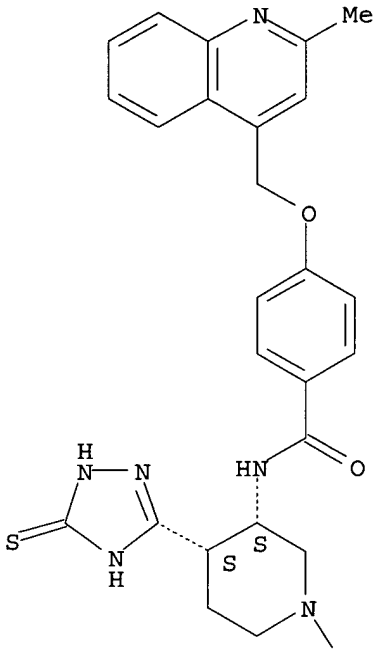
CM 1

CRN 681284-99-1
CMF C25 H26 N6 O2 S

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

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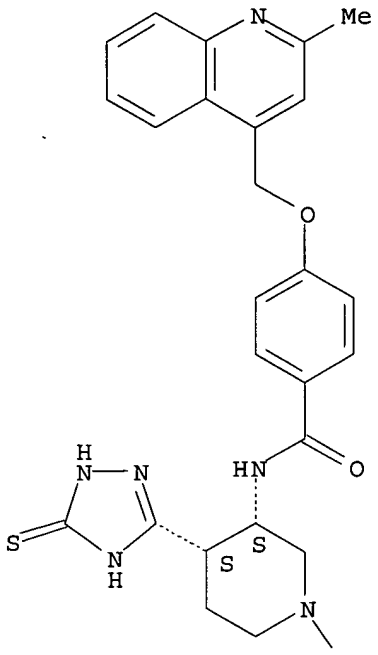
CN Benzamide, N-[(3S,4S)-1-acetyl-4-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3-piperidinyl]-4-[(2-methyl-4-quinolinyl)methoxy]-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 681285-02-9
CMF C27 H28 N6 O3 S

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

Pr-n

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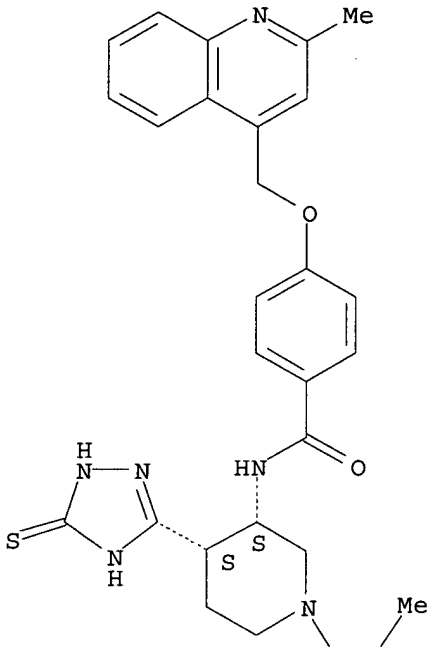
CM 1

CRN 681285-05-2
CMF C28 H32 N6 O2 S

Absolute stereochemistry.

PAGE 1-A



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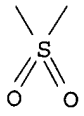

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CM 1

CRN 681285-16-5
CMF C26 H28 N6 O4 S2

Absolute stereochemistry.

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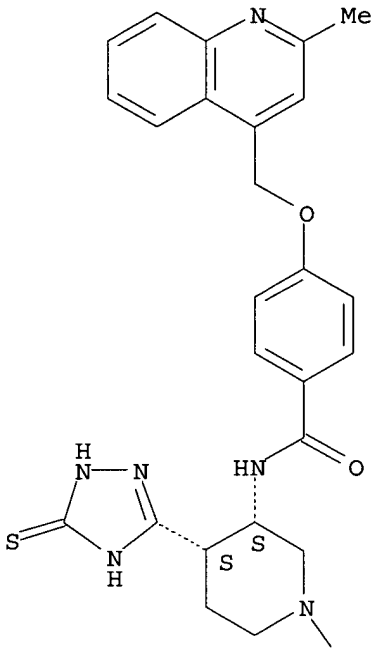

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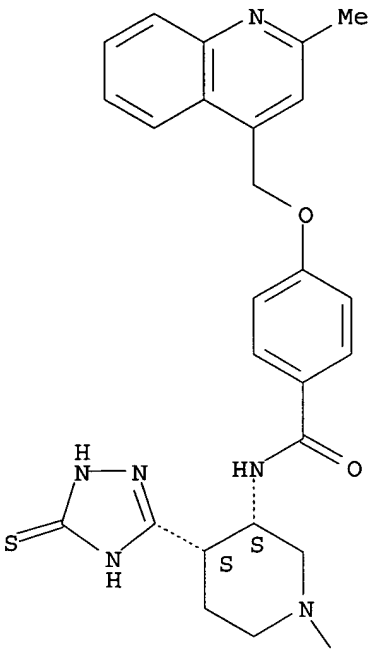
CM 1

CRN 681285-21-2
CMF C28 H32 N6 O2 S

Absolute stereochemistry.

PAGE 1-A



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RN 681285-35-8 HCAPLUS
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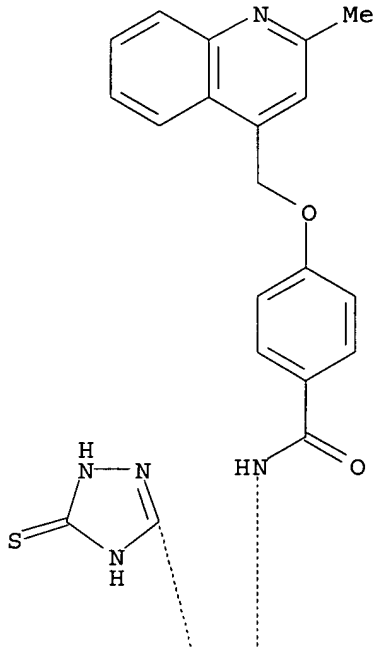
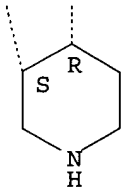
Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



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CRN 76-05-1
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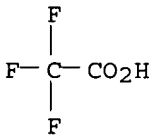
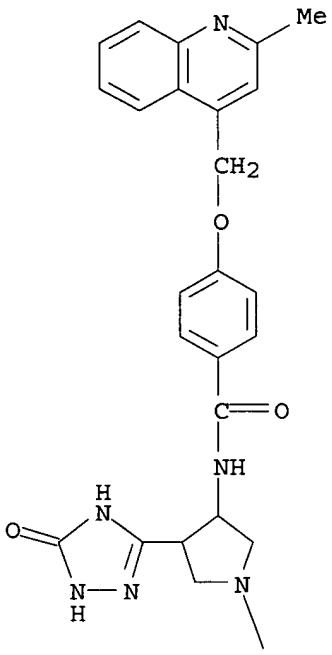
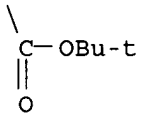


RN 681285-43-8 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 3-(2,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl)-4-[[4-[(2-methyl-4-quinolinyl)methoxy]benzoyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

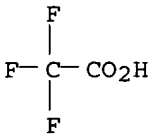


PAGE 2-A



CM 2

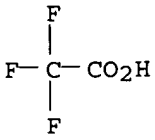
CRN 76-05-1
CMF C2 H F3 O2



RN 681285-46-1 HCAPLUS
CN Benzamide, N-[3-(2,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl)tetrahydro-2H-pyran-4-yl]-4-[(2-methyl-4-quinolinyl)methoxy]- (9CI) (CA INDEX NAME)

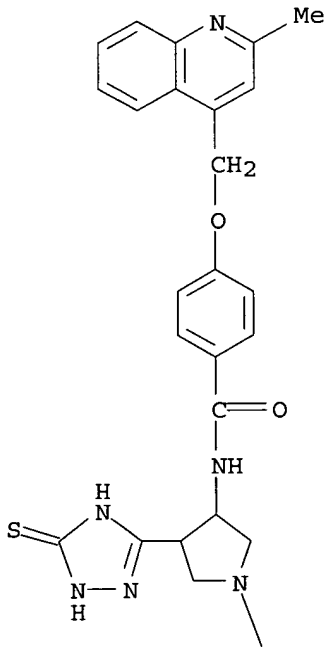
CM 2

CRN 76-05-1
CMF C2 H F3 O2

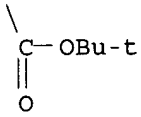


RN 681285-51-8 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 3-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-4-[[4-[(2-methyl-4-quinolinyl)methoxy]benzoyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

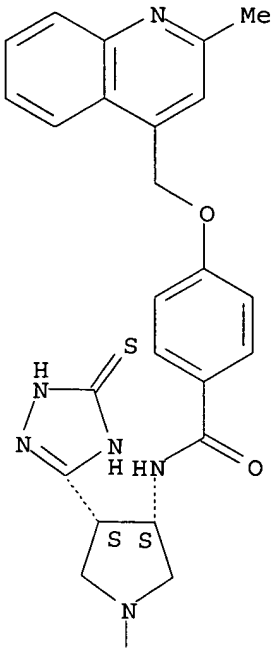


PAGE 2-A



RN 681285-52-9 HCAPLUS
CN Benzamide, N-[4-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3-pyrrolidinyl]-4-[(2-methyl-4-quinolinyl)methoxy]- (9CI) (CA INDEX NAME)

PAGE 1-A



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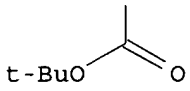
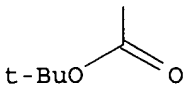


RN 681284-69-5 HCAPLUS
CN Benzamide, N-[(3S,4S)-4-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3-pyrrolidinyl]-4-[(2-methyl-4-quinolinyl)methoxy]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 2-A

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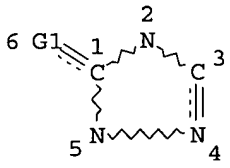


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DEFAULT ECLEVEL IS LIMITED

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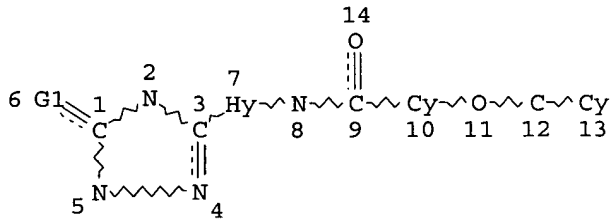


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L13            1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12
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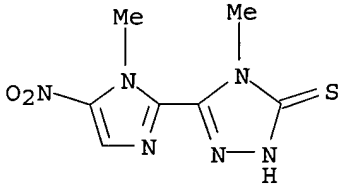
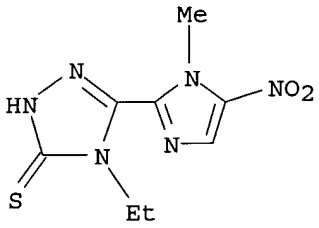
significant effects against Bacillus subtilis at MIC ranges of 0.5-1 μg/mL and moderate effects against Staphylococcus aureus.

IT **590367-76-3P 590367-77-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and in vitro antimicrobial and antifungal evaluation of 5-(1-methyl-5-nitro-2-imidazolyl)-4H-1,2,4-triazoles)

RN 590367-76-3 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 2,4-dihydro-4-methyl-5-(1-methyl-5-nitro-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)



RN 590367-77-4 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 4-ethyl-2,4-dihydro-5-(1-methyl-5-nitro-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)

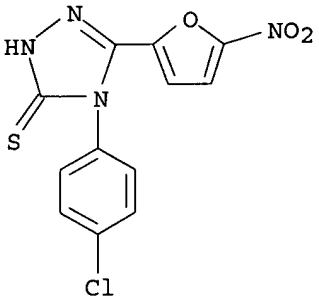


REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:5774 HCAPLUS
DOCUMENT NUMBER: 138:66658
TITLE: Novel nitrofuran-containing heterocyclic compounds and uses thereof
INVENTOR(S): Magee, Andrew S.; Roy, Aloka; Moe, Scott T.; Griffith, Jim P.; Ala, Paul J.; Ali, Janid; Clement, Jacob J.; Navia, Manuel
PATENT ASSIGNEE(S): Essential Therapeutics, Inc., USA; Pliva D.D.
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2003000255 | A1 | 20030103 | WO 2002-US20387 | 20020625 <-- |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

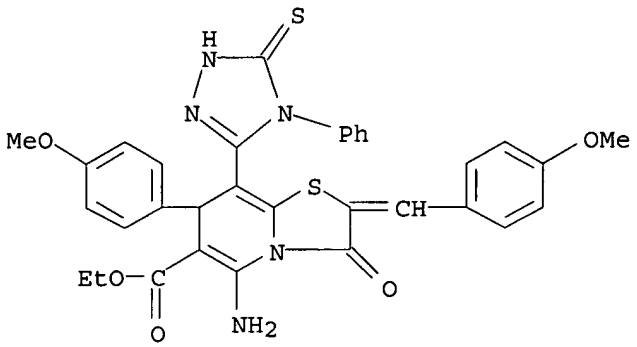
L22 ANSWER 3 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:217205 HCAPLUS
DOCUMENT NUMBER: 137:352962
TITLE: Synthesis of some new triazoles as potential antifungal agents
AUTHOR(S): Fahmy, Hesham T. Y.
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Alexandria, Alexandria, Egypt
SOURCE: Bollettino Chimico Farmaceutico (**2001**), 140(6), 422-427
CODEN: BCFAAI; ISSN: 0006-6648
PUBLISHER: Societa Editoriale Farmaceutica
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:352962

AB The rise in the incidence of fungal infections over the past two decades, particularly those caused by opportunistic pathogens in immune-compromised patients, has strengthened the need for new antifungal drugs. New triazole derivs. were synthesized and evaluated for their in-vitro antifungal activities against three species of fungi. Most of the prepared compds. showed good antifungal activity. Three compds. exhibited pronounced activity against Cryptococcus neoformans with MIC less than 12.5 g/mL.

IT **474971-94-3P 474971-99-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antifungal activity of substituted triazoles)

RN 474971-94-3 HCAPLUS
CN 7H-Thiazolo[3,2-a]pyridine-6-carbonitrile, 5-amino-7-(4-chlorophenyl)-2-[(4-chlorophenyl)methylene]-8-(4,5-dihydro-4-phenyl-5-thioxo-1H-1,2,4-triazol-3-yl)-2,3-dihydro-3-oxo- (9CI) (CA INDEX NAME)

phenyl-5-thioxo-1H-1,2,4-triazol-3-yl)-2,3-dihydro-7-(4-methoxyphenyl)-2-[(4-methoxyphenyl)methylene]-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



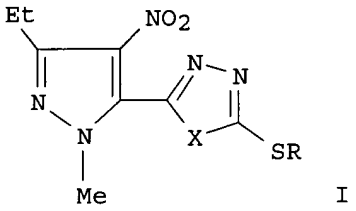
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:693264 HCAPLUS
DOCUMENT NUMBER: 135:257269
TITLE: Preparation of N-heterocyclyl amide compounds as 5-HT antagonists
INVENTOR(S): Yamada, Akira; Tomishima, Masaki; Hayashida, Hisashi; Imanishi, Masashi; Spears, Glen W.; Ito, Kiyotaka; Takahashi, Fumie; Miyake, Hiroshi
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 239 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001068585 | A1 | 20010920 | WO 2001-JP1993 | 20010313 <-- |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2001041128 | A5 | 20010924 | AU 2001-41128 | 20010313 <-- |
| EP 1264820 | A1 | 20021211 | EP 2001-912338 | 20010313 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| US 2004087798 | A1 | 20040506 | US 2002-221554 | 20021227 |
| PRIORITY APPLN. INFO.: | | | JP 2000-70127 A | 20000314 |
| | | | JP 2000-305947 A | 20001005 |
| | | | WO 2001-JP1993 W | 20010313 |

OTHER SOURCE(S): CASREACT 135:257269; MARPAT 135:257269
AB Amides compds. represented by the general formula R1-A-X-NHCO-Y-R2 [wherein R1 is an optionally substituted heterocyclic group or optionally substituted phenyl; R2 is optionally substituted fused Ph, optionally

ACCESSION NUMBER: 2001:491585 HCAPLUS
DOCUMENT NUMBER: 135:210994
TITLE: Synthesis of pyrazolylheterocycles and their fungicidal activities
AUTHOR(S): Zhao, Wei-Guang; Chen, Han-Song; Li, Zheng-Ming; Han, Yu-Fen; Yan, Han; Lai, Jun-Ying; Wang, Su-Hua
CORPORATE SOURCE: Institute of Elemento-organic Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (**2001**), 22(6), 939-942
CODEN: KTHPDM; ISSN: 0251-0790
PUBLISHER: Gaodeng Jiaoyu Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 135:210994
GI

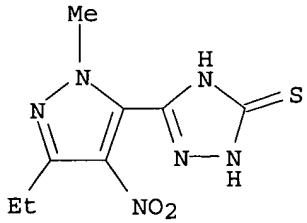


I

AB Title compds. I (R = CH3, CH3CH2, CH2CH:CH2, CH2CO2CH2CH3, CH2C6H5; X = O, S, NH) were prepared from 1-methyl-3-ethyl-4-nitropyrazolylcarboxylic acid. The structures of all new compds. were confirmed by 1H NMR and elementary anal. Their fungicidal activity was evaluated against Rhizoctonia solani. Structure-activity relationships for the screened compds. were evaluated and discussed. It was found that some compds. showed a higher fungicidal activity and systematic activity.

IT **358641-26-6P 358641-27-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and fungicidal activities of pyrazolylheterocycles)

RN 358641-26-6 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(3-ethyl-1-methyl-4-nitro-1H-pyrazol-5-yl)-1,2-dihydro- (9CI) (CA INDEX NAME)



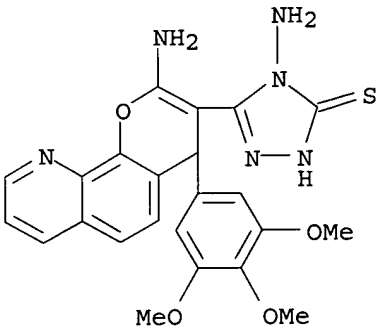
RN 358641-27-7 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(3-ethyl-1-methyl-4-nitro-1H-pyrazol-5-yl)-2,4-dihydro-4-phenyl- (9CI) (CA INDEX NAME)

reaction of the carboxyhydrazide with Ph isothiocyanate, acetylacetone, and benzoylacetone resulted in the formation of II and III (R = Me, Ph), resp. Et carbazate as a typical mesophile reacted with I (R = COOEt) to afford a fused tetracyclic product, a triazepinopyranoquinoline, via cyclization of the initially formed hydrazide. Among sixteen compds. screened against E. coli and S. aureus, two compds. show a high order of antibacterial activity against both bacteria. IV is strongly potent against Staphylococcus aureus.

IT **389636-95-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antibacterial activity of 4H-pyrano[3,2-h]quinolines and fused derivs.)

RN 389636-95-7 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 4-amino-5-[2-amino-4-(3,4,5-trimethoxyphenyl)-4H-pyrano[3,2-h]quinolin-3-yl]-2,4-dihydro- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 7 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:334876 HCAPLUS

DOCUMENT NUMBER: 135:122486

TITLE: Heteroaromatization with ketene dithioacetals: Part I. Synthesis of some novel 5-amino-1-(1,3,4-thiadiazol-2-yl) and 1-(1,3,4-thiadiazin-2-yl)pyrazole-4-carbonitriles

AUTHOR(S): Hassan, Saber M.; Emam, Hussein A.; Abdelall, Mahmoud M.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Al-Azhar University, Cairo, 11884, Egypt

SOURCE: Journal of Chemical Research, Synopses (**2000**), (12), 544-545, 1301-1315
CODEN: JRPSDC; ISSN: 0308-2342

PUBLISHER: Science Reviews Ltd.

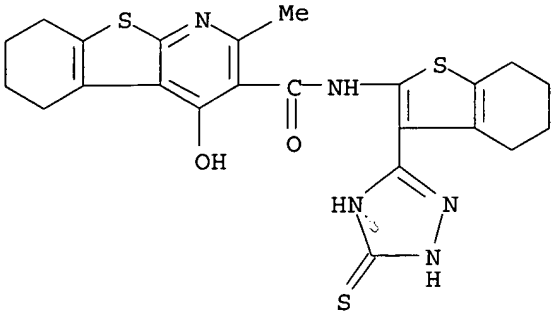
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:122486

AB 5-Amino-3-methylthio-1-(1,3,4-thiadiazol-2-yl) and 1-(1,3,4-thiadiazin-2-yl)pyrazole-4-carbonitriles were prepared from 5-aminopyrazoles using ketene dithioacetals as starting materials. For example, (MeS)2C:C(CN)2 and (H2NNH)2C:S refluxed in EtOH gave 75% 1-(5-amino-4-cyano-3-methylthiopyrazol-1-yl)carbothiohydrazide (2a); 2a with PhCO2H and POCl3 gave 65% 5-benzoylamino-3-methylthio-1-(5-phenyl-1,3,4-thiadiazol-2-yl)pyrazole-4-carbonitrile. 2A, chloroacetic acid and NaOAc in refluxing EtOH gave 66% 5-amino-3-methylthio-1-(5-oxo-1,3,4-thiadiazin-2-yl)pyrazole-

CN [1]Benzothieno[2,3-b]pyridine-3-carboxamide, N-[3-(2,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]-5,6,7,8-tetrahydro-4-hydroxy-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 9 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:631584 HCAPLUS
DOCUMENT NUMBER: 132:49927
TITLE: Synthesis, characterization and evaluation of the activity of ten mesoionic compounds against microorganisms
AUTHOR(S): De Athayde-Filho, Petronio Filgueiras; Miller, Joseph; Simas, Alfredo Mayall.; De Sena, Kesia Xisto da Fonseca Ribeiro; Chiappeta, Alda de Andrade
CORPORATE SOURCE: Departamento de Quimica, Universidade Federal Rural de Pernambuco, Recife-PE, 52.171-030, Brazil
SOURCE: Acta Farmaceutica Bonaerense (**1999**), 18(1), 17-22
CODEN: AFBODJ; ISSN: 0326-2383
PUBLISHER: Colegio de Farmaceuticos de la Provincia de Buenos Aires
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three mesoionic 1,3,4-thiadiazolium-2-thiolates and seven 1,3,4-triazolium-2-thiol chlorides have been synthesized and tested for activity against a range of microorganisms. The chemical structures were confirmed by elemental anal., IR, mass, 1H and 13C NMR spectrometry. The biol. tests indicate that the compds. have substantial activity against Gram-pos. and alc.-acid-resistant bacteria; moderate activity against yeasts and little activity against other fungi and are inactive against Gram-neg. bacteria.
IT **187875-14-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal and fungicidal activity of thiadiazoliumthiolates and triazoliumthiol chlorides)
RN 187875-14-5 HCAPLUS
CN 1H-1,2,4-Triazolium, 4,5-dihydro-3-(5-nitro-2-furanyl)-2,4-diphenyl-5-thioxo-, chloride (9CI) (CA INDEX NAME)

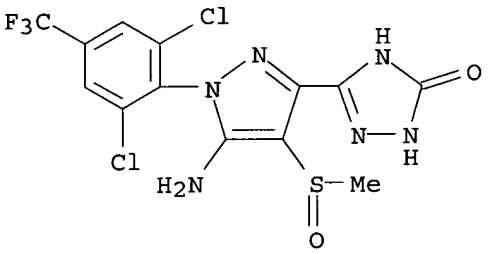
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; R1 = II-IV (R1a = H, alkyl, a lone pair of electrons; R1b = alkyl, aryl; X = O, NH, N(alkyl); Q = CR8R9, C(:Y), etc.; R8, R9 = H, alkyl, aryl, etc.; Y = O, S; Z = alkyl, aryl; W = H, alkyl, alkenyl, etc.; V = H, alkyl, CN, etc.); R2 = alkyl, haloalkyl, SOnR2a (R2a = alkyl, alkenyl, alkynyl, etc.); R3 = H, halo, alkyl, etc.; R4, R5, R7 = H, halo, alkyl; R6 = halo, haloalkyl, haloalkoxy, etc.; M = C(halo), C(Me), N, etc.], having pesticidal activity, were prepared Thus, reaction of 5-amino-1-(2,6-dichloro-4-trifluoromethylphenyl)-4-methylsulfinyl-3-[3-(1-amidoxime)]pyrazole (preparation given) with trifluoroacetic anhydride in dioxane afforded the title compound V which showed insecticidal activity in one or more of the evaluation methods (described in patent), with particularly good activity in the systemic tests.

IT **223582-94-3P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pesticidal 3-substituted arylpyrazoles)

RN 223582-94-3 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 5-[5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(methylsulfinyl)-1H-pyrazol-3-yl]-1,2-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 11 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:424251 HCAPLUS
DOCUMENT NUMBER: 129:95500
TITLE: Preparation of 2-(1,2,4-triazol-3-ylthio)-, 2-(5-tetrazolylthio)-, 2-(1,3,4-thiadiazol-2-ylthio)thiazole compounds and methods of modulating signal transduction
INVENTOR(S): Tang, Peng C.; Ramphal, John Y.; Harris, G. Davis, Jr.; Nematalla, Asaad S.
PATENT ASSIGNEE(S): Sugen, Inc., USA
SOURCE: PCT Int. Appl., 175 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

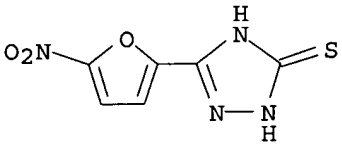
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|

cancer, colon cancer, or epidermoid cancer, and diabetes mellitus. Thus, 2-bromo-5-nitrothiazole was condensed with 4-[4-(4,5-dichloroimidazol-1-yl)phenyl]-2-mercaptopyrimidine at room temperature for 24 h to give the title compound, 4-(imidazolylphenyl)-2-(thiazolylthio)pyrimidine (II). In a phosphotyrosine enzyme linked immunosorbent assay, II inhibited dephosphorylation of phosphotyrosine residues on insulin receptor in NIH3T3 cells engineered to over-express the human insulin receptor (H25 cells) with EC50 (50% increase in the amount of phosphotyrosine over the control) of 3 μM.

IT **57672-16-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiazole compds. modulating signal transduction as tyrosine phosphatase inhibitors for treatment of diseases)

RN 57672-16-9 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 1,2-dihydro-5-(5-nitro-2-furanyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 12 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:391083 HCAPLUS

DOCUMENT NUMBER: 129:175593

TITLE: Synthesis, antifungal and antibacterial activity of substituted 1,2,4-triazoles

AUTHOR(S): Pourmorad, F.; Shafiee, A.

CORPORATE SOURCE: Department of Chemistry, Faculty of Pharmacy, The Medical Sciences University of Tehran, Tehran, Iran

SOURCE: Journal of Sciences, Islamic Republic of Iran (**1998**), 9(1), 30-33
CODEN: JSIIEN; ISSN: 1016-1104

PUBLISHER: National Center for Scientific Research

DOCUMENT TYPE: Journal

LANGUAGE: English

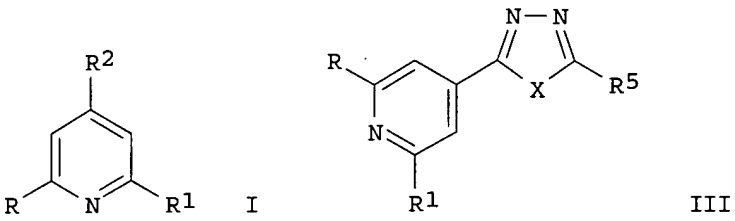
AB The reaction of readily available 1-methyl-4-nitropyrrole-2-carboxylic acid with thionyl chloride afforded the corresponding carbonyl chloride. The reaction of the latter with thiosemicarbazides yielded 1-(1-methyl-4-nitropyrrole-2-carbonyl)thiosemicarbazides which cyclized in basic medium to 5-(1-methyl-4-nitropyrrole-2-yl)-2,4-dihydro-3H-1,2,4-triazole-3-thione derivs. Alkylation the latter and subsequent oxidation of (pyrrolyl)-1,2,4-triazoles. The antibacterial and antifungal activities of these against a number of microorganisms were determined Only two compds. had moderate activity against Aspergillus niger.

IT **211626-82-3P 211626-83-4P 211626-84-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and antifungal and antibacterial activity of (pyrrolyl)-1,2,4-triazoles)

RN 211626-82-3 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 2,4-dihydro-5-(1-methyl-4-nitro-1H-pyrrol-2-yl)-4-phenyl- (9CI) (CA INDEX NAME)

GI



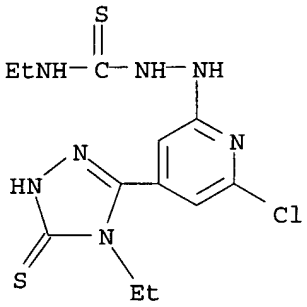
I III

AB Condensation of pyridines I (R = R1 = OH, R = Cl, R1 = NHNH2, R2 = CONHNH2) (II) with R3CHO (R3 = Ph, 2,4-(OH)C6H3, 2-thienyl, 4-pyridyl, 4-Me2NC6H4) gave 35-87% I (R, R1 = same as above, R2 = CONHN:CHR3) and reactions of II with R4NCX (R4 = Ph, Et; X = O, S) gave 31-89% I (R = Cl, OH; R1 = OH, NHNHC(X)NHR4, R2 = CONHNHC(X)NHR4), which cyclized to give 38-68% III (R = Cl, OH; R1 = OH, NHNHC(X)NHR4, R5 = XH, NHR4, X = O, S, NR4). Compds. I (R = R1 = OH, R2 = CONHN:CHPh) and III (R = R1 = OH, R5 = SH, X = NEt) were more effective as bactericides against Bacillus subtilis than ampicillin.

IT **197902-02-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and microbicidal activity of)

RN 197902-02-6 HCAPLUS

CN Hydrazinecarbothioamide, 2-[6-chloro-4-(4-ethyl-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-2-pyridinyl]-N-ethyl- (9CI) (CA INDEX NAME)



IT **197901-99-8P 197902-00-4P 197902-03-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 197901-99-8 HCAPLUS

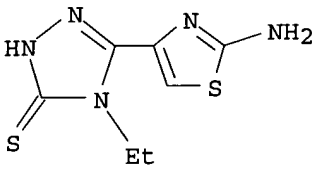
CN Hydrazinecarboxamide, 2-[6-chloro-4-(4-ethyl-4,5-dihydro-5-oxo-1H-1,2,4-triazol-3-yl)-2-pyridinyl]-N-ethyl- (9CI) (CA INDEX NAME)

CORPORATE SOURCE: Dep. Medicinal Chem., Fac. Pharmacy, Univ. Mansoura, Mansoura, 35516, Egypt
SOURCE: Qatar University Science Journal (**1994**), 14(Spec. Issue), 55-60
CODEN: QUSJEV; ISSN: 1023-8948
PUBLISHER: University of Qatar, Faculty of Science
DOCUMENT TYPE: Journal
LANGUAGE: English

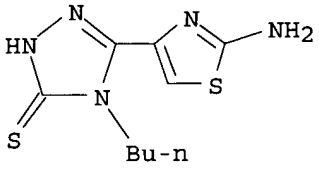
AB A series of thiazole derivs. bearing amino, acetamido or thioureido synthons at position 2 and thiosemicarbazone or 1,2,4-triazolethione moieties at position 4 have been synthesized and evaluated for their antimicrobial and antitumor activities. Some of the tested compds. proved to possess a remarkable antitumor antibiotic activity. The antimicrobial potency is found mainly to be against Gram pos. bacteria. The detailed synthesis, spectroscopic, and biol. data are reported.

IT **157521-62-5P 157521-63-6P 157521-64-7P**
**157521-65-8P 157521-66-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and antimicrobial and antitumor activities of thiazoles)

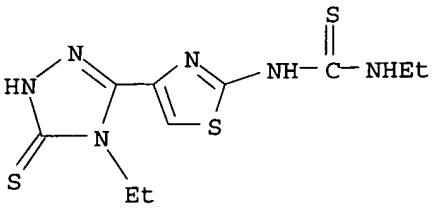
RN 157521-62-5 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-ethyl-2,4-dihydro- (9CI) (CA INDEX NAME)



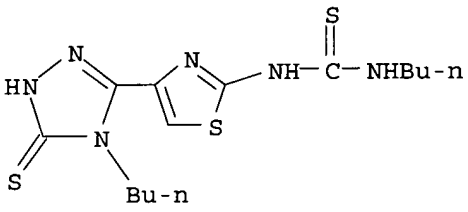

RN 157521-63-6 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-butyl-2,4-dihydro- (9CI) (CA INDEX NAME)



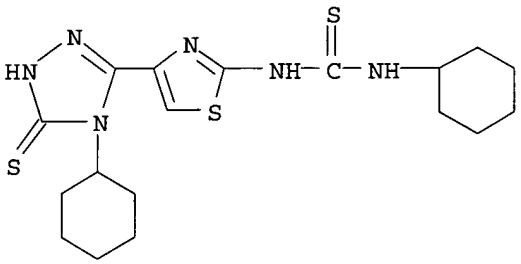

RN 157521-64-7 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-cyclohexyl-2,4-dihydro- (9CI) (CA INDEX NAME)



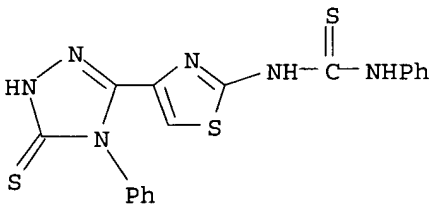
RN 157521-73-8 HCAPLUS
CN Thiourea, N-butyl-N'-[4-(4-butyl-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



RN 157521-74-9 HCAPLUS
CN Thiourea, N-cyclohexyl-N'-[4-(4-cyclohexyl-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



RN 157521-75-0 HCAPLUS
CN Thiourea, N-[4-(4,5-dihydro-4-phenyl-5-thioxo-1H-1,2,4-triazol-3-yl)-2-thiazolyl]-N'-phenyl- (9CI) (CA INDEX NAME)

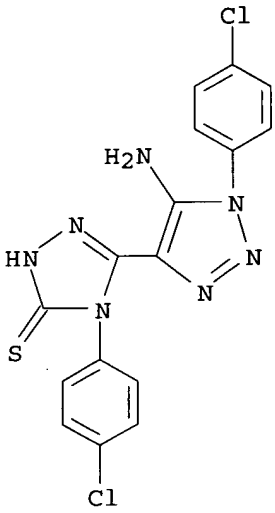


RN 157521-76-1 HCAPLUS
CN Thiourea, N-(4-fluorophenyl)-N'-[4-[4-(4-fluorophenyl)-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl]-2-thiazolyl]- (9CI) (CA INDEX NAME)

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of)

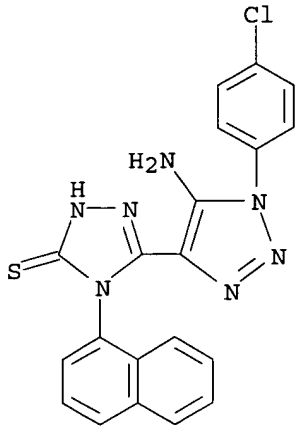
RN 188559-81-1 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-4-(4-chlorophenyl)-2,4-dihydro- (9CI) (CA INDEX NAME)




RN 188559-85-5 HCAPLUS

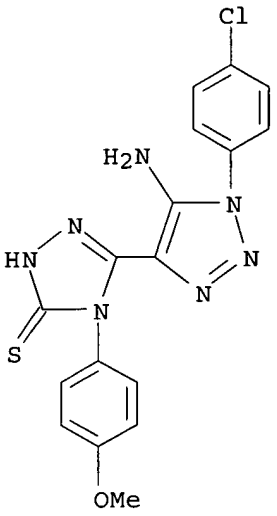
CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-2,4-dihydro-4-(1-naphthalenyl)- (9CI) (CA INDEX NAME)



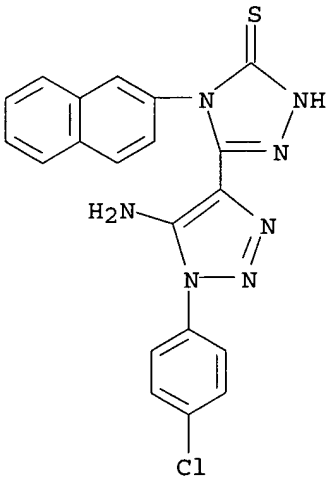

IT **188559-80-0P 188559-82-2P 188559-84-4P**
**188559-86-6P 188559-87-7P 188559-88-8P**
**188559-89-9P 188559-90-2P 188559-91-3P**
**188559-92-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 188559-80-0 HCAPLUS

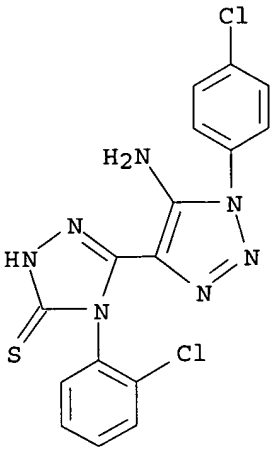
CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-2,4-dihydro-4-phenyl- (9CI) (CA INDEX NAME)



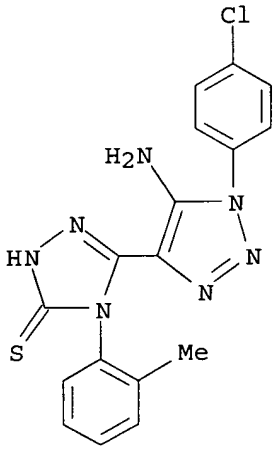

RN 188559-86-6 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-2,4-dihydro-4-(2-naphthalenyl)- (9CI) (CA INDEX NAME)




RN 188559-87-7 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-4-(4-ethoxyphenyl)-2,4-dihydro- (9CI) (CA INDEX NAME)

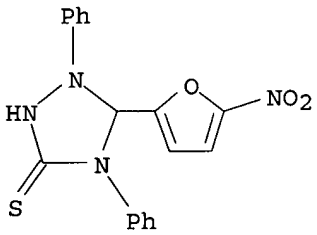


RN 188559-90-2 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-2,4-dihydro-4-(2-methylphenyl)- (9CI) (CA INDEX NAME)



RN 188559-91-3 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-[5-amino-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-2,4-dihydro-4-(3-methylphenyl)- (9CI) (CA INDEX NAME)

PUBLISHER: Freund
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Mesoionic 1,4-diphenyl-5-(5-nitro-2-furanyl)-1,3,4-triazolium-2-thiolate was prepared as its hydrochloride by the reaction of 1,4-diphenylthiosemicarbazide with 5-nitro-2-furoyl chloride. The structure was confirmed by elemental anal., IR, mass, 1H and 13C NMR spectra. Pharmacol. tests in vitro showed that the compound possesses spasmolytic action in the guinea-pig trachea and the rat uterus, but not in the guinea-pig ileum.
IT **187875-14-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and spasmolytic activity of diphenylnitrofuranyltriazoliumthiolate)
RN 187875-14-5 HCAPLUS
CN 1H-1,2,4-Triazolium, 4,5-dihydro-3-(5-nitro-2-furanyl)-2,4-diphenyl-5-thioxo-, chloride (9CI) (CA INDEX NAME)




● Cl⁻

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L22 ANSWER 17 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:42600 HCAPLUS
DOCUMENT NUMBER: 126:186026
TITLE: Synthesis and biological studies of bis-heterocycles
AUTHOR(S): Kudari, S. M.; Beede, S. M.; Munera, Wahaja
CORPORATE SOURCE: Dep. Chem., Gulbarga Univ., Gulbarga, 585 106, India
SOURCE: Asian Journal of Chemistry (**1997**), 9(1), 20-26
CODEN: AJCHEW; ISSN: 0970-7077
PUBLISHER: Asian Journal of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

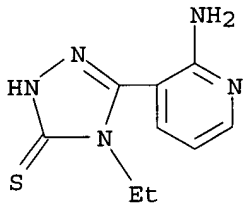
L22 ANSWER 18 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:161585 HCAPLUS
DOCUMENT NUMBER: 124:220521
TITLE: Cytoprotection utilizing aryltriazol-3-thiones
INVENTOR(S): Connor, David T.; Plummer, Janet S.
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 5489598 | A | 19960206 | US 1994-255597 | 19940608 <-- |
| PRIORITY APPLN. INFO.: | | | US 1994-255597 | 19940608 |

OTHER SOURCE(S): MARPAT 124:220521

AB 5-Aryltriazol-3-thiones are useful for inhibiting adhesion of Mac-1 to the endothelium and thereby providing cytoprotection for diseases mediated by Mac-1 adhesion, such as nonsteroidal anti-inflammatory drug-induced gastritis, inflammatory bowel disease, and ulcerative colitis. The compds. were prepared and evaluated for inhibitory activity against Mac-1 adhesion in in vitro and in vivo models. For example, 5-(2-amino-5-chlorophenyl)-4-ethyl-2,4-dihydro-[1,2,4]triazol-3-thione inhibited the adhesion of Mac-1 to keyhole limpet hemocyanin-coated plates in vitro and prevented the aspirin-induced gastric damage in rats.

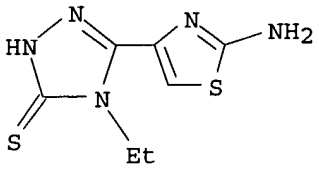
IT **174573-81-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(aryltriazol-3-thiones for inhibition of Mac-1 adhesion to endothelial cells for treatment of gastritis and colitis)
RN 174573-81-0 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-3-pyridinyl)-4-ethyl-2,4-dihydro- (9CI) (CA INDEX NAME)



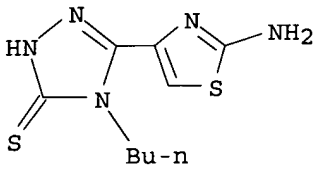

L22 ANSWER 19 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:557485 HCAPLUS
DOCUMENT NUMBER: 121:157485
TITLE: Synthesis of some 2-(substituted thio)pyridines and thieno[2,3-b]pyridines
AUTHOR(S): Abdel-Monem, Maisa I.
CORPORATE SOURCE: Fac. Sci., Assiut Univ., Assiut, 71516, Egypt
SOURCE: Collection of Czechoslovak Chemical Communications ( **1994**), 59(4), 978-86
CODEN: CCCCAK; ISSN: 0010-0765

**157521-76-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antibacterial and antitumor activities of, structure in relation to)

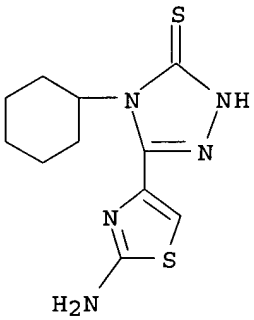
RN 157521-62-5 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-ethyl-2,4-dihydro- (9CI) (CA INDEX NAME)



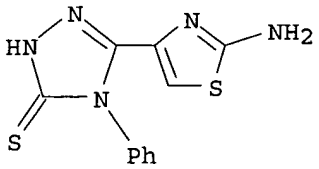
RN 157521-63-6 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-butyl-2,4-dihydro- (9CI) (CA INDEX NAME)

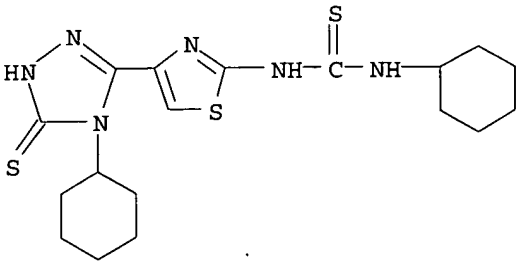


RN 157521-64-7 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-4-cyclohexyl-2,4-dihydro- (9CI) (CA INDEX NAME)

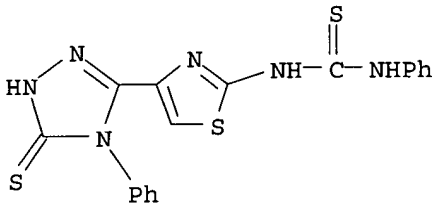


RN 157521-65-8 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(2-amino-4-thiazolyl)-2,4-dihydro-4-phenyl- (9CI) (CA INDEX NAME)

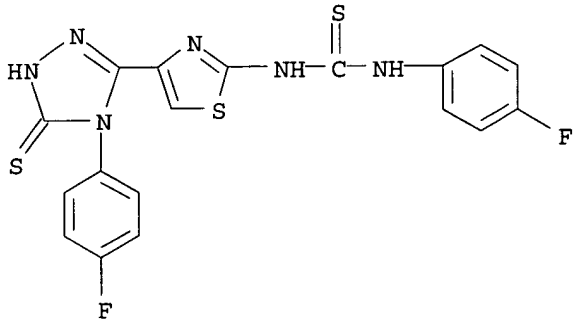




RN 157521-75-0 HCAPLUS
CN Thiourea, N-[4-(4,5-dihydro-4-phenyl-5-thioxo-1H-1,2,4-triazol-3-yl)-2-thiazolyl]-N'-phenyl- (9CI) (CA INDEX NAME)

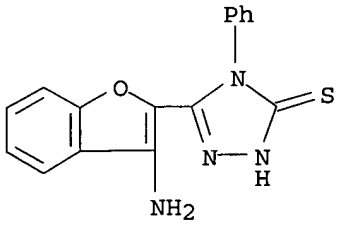


RN 157521-76-1 HCAPLUS
CN Thiourea, N-(4-fluorophenyl)-N'-[4-[4-(4-fluorophenyl)-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl]-2-thiazolyl]- (9CI) (CA INDEX NAME)

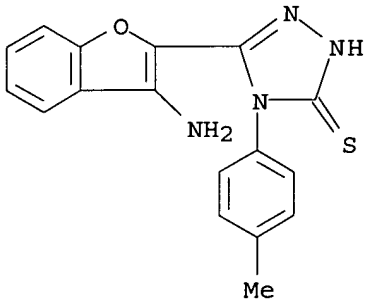


L22 ANSWER 21 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

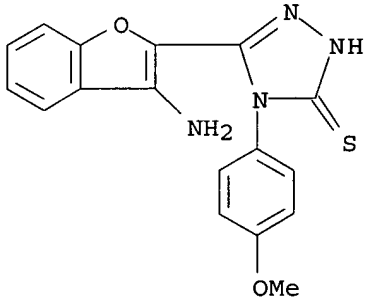
| | |
|---|---|
| ACCESSION NUMBER: | 1993:22188 HCAPLUS |
| DOCUMENT NUMBER: | 118:22188 |
| TITLE: | Synthesis of 1,3,4-oxadiazolyl, thiadiazolyl and 1,2,4-triazolyl-3-aminobenzofurans and related compounds |
| AUTHOR(S): | Basavaraja, K. M.; Vaidya, V. P.; Sangapure, S. S.; Agasimundin, Y. S. |
| CORPORATE SOURCE: | Dep. Chem., Gulbarga Univ., Gulbarga, 585 106, India |
| SOURCE: | Indian Journal of Heterocyclic Chemistry (**1992**), 2(1), 35-40<br>CODEN: IJCHEI; ISSN: 0971-1627 |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | English |




RN 144990-19-2 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(3-amino-2-benzofuranyl)-2,4-dihydro-4-(4-methylphenyl)- (9CI) (CA INDEX NAME)

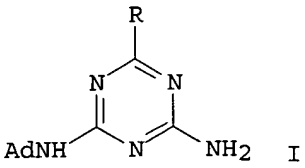



RN 144990-20-5 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(3-amino-2-benzofuranyl)-2,4-dihydro-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)




RN 144990-21-6 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(3-amino-2-benzofuranyl)-4-(4-chlorophenyl)-2,4-dihydro- (9CI) (CA INDEX NAME)

OTHER SOURCE(S): CASREACT 117:69834
GI



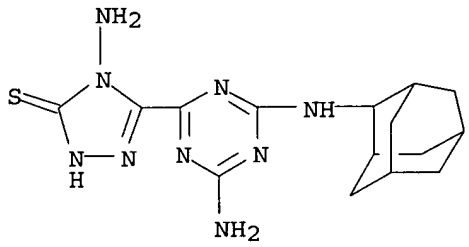
I

AB (Adamantylamino)triazines I [Ad = 2-adamantyl, R = CONHNHC(Z)NHR1 (Z = O, R1 = Pr, Ph; Z = S, R1 = alkyl, aryl, Ad)] and their cyclization products I (R = 4-R1-substituted-5-hydroxy(or mercapto)-1,2,4-triazol-3-yl) were prepared from hydrazide I (R = CONHNH2) and iso(thio)cyanates RNCZ. Cyclocondensation reactions were also carried out between the hydrazide and CS2 or CS2-N2H4-HCO2Et to give I (R = 5-mercapto-1,3,4-oxadiazol-2-yl) and I (R = 1,2,4-triazolo[5,4-b]-1,3,4-thiadiazol-3-yl), resp.

IT **142530-46-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with formate)

RN 142530-46-9 HCAPLUS

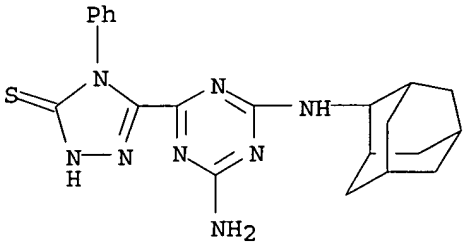
CN 3H-1,2,4-Triazole-3-thione, 4-amino-5-[4-amino-6-(tricyclo[3.3.1.13,7]dec-2-ylamino)-1,3,5-triazin-2-yl]-2,4-dihydro- (9CI) (CA INDEX NAME)



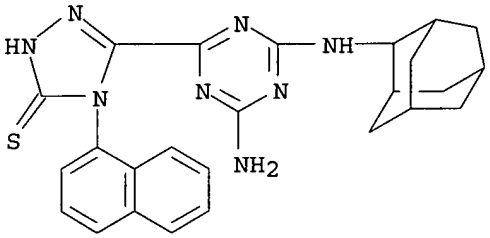

IT **142530-35-6P 142530-36-7P 142530-37-8P**
**142530-38-9P 142530-39-0P 142530-40-3P**
**142530-41-4P 142530-42-5P 142530-43-6P**
**142530-44-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 142530-35-6 HCAPLUS

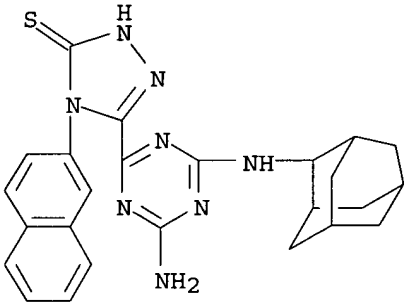
CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-(tricyclo[3.3.1.13,7]dec-2-ylamino)-1,3,5-triazin-2-yl]-2,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)



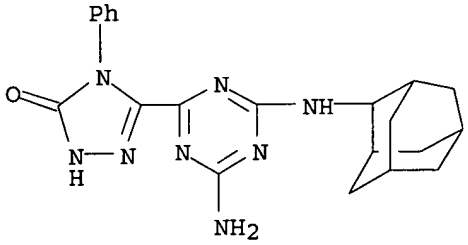
RN 142530-39-0 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-(tricyclo[3.3.1.13,7]dec-2-ylamino)-1,3,5-triazin-2-yl]-2,4-dihydro-4-(1-naphthalenyl)- (9CI) (CA INDEX NAME)



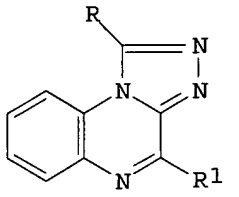
RN 142530-40-3 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-(tricyclo[3.3.1.13,7]dec-2-ylamino)-1,3,5-triazin-2-yl]-2,4-dihydro-4-(2-naphthalenyl)- (9CI) (CA INDEX NAME)



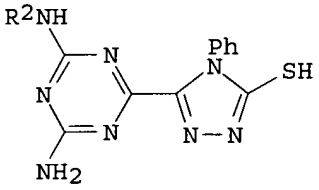
RN 142530-41-4 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-(tricyclo[3.3.1.13,7]dec-2-ylamino)-1,3,5-triazin-2-yl]-4-(4-fluorophenyl)-2,4-dihydro- (9CI) (CA INDEX NAME)



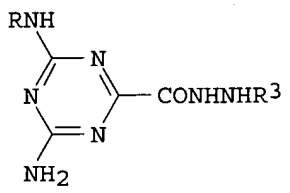
L22 ANSWER 23 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:59325 HCAPLUS
DOCUMENT NUMBER: 116:59325
TITLE: Synthesis and characterization of 1,2,4-triazolo[4,3-a]quinoxalines and 1,2,4-triazolo-s-triazines as potential antimicrobial agents
AUTHOR(S): El-Kerdawy, M.; Tantawy, A.; Gad, L. M.; Rady, E.
CORPORATE SOURCE: Fac. Pharm., Univ. Mansoura, Mansoura, Egypt
SOURCE: Zhonghua Yaoxue Zazhi (**1991**), 43(5), 355-64
CODEN: CYHCEX; ISSN: 1016-1015
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



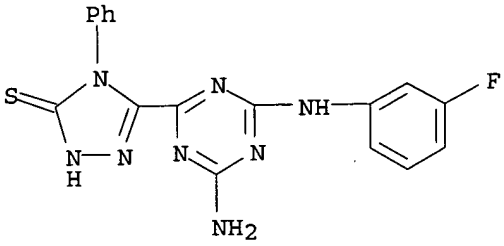
II



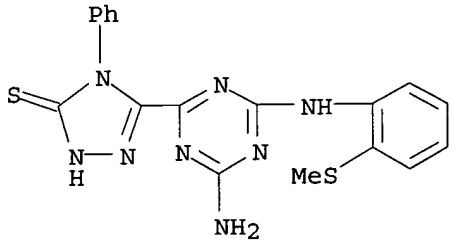
III

AB Several triazoloquinoxalines were synthesized via a series of reactions. Condensation of 2-chloro-3-hydrazinoquinoxaline with different aromatic aldehydes gave the corresponding hydrazones, which were directly cyclized to 4-chloro-1-aryl-1,2,4-triazolo[4,3-a]quinoxalines I (R = 4-BrC6H4, 2-ClC6H4, 4-ClC6H4; R1 = Cl) in bromine/acetic acid. Subsequent displacement of the very reactive chloro substituent by a variety of nucleophiles was performed to yield 4-alkoxy and 4-substituted amino derivs. I (R1 = OMe, OEt, morpholino, piperidino). Several s-triazole derivs. II (R2 = 2-FC6H4, 2-MeSC6H4, 2-MeOC6H4) were prepared through the cyclization of the corresponding 4-amino-6-substituted anilino-s-triazine-2-carboxyhydrazides III (R3 = H) using Ph isothiocyanate in alkaline medium, or by refluxing 1-phenyl-4-(4-amino-6-

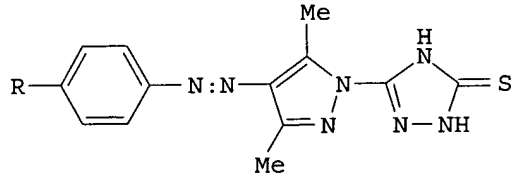
RN 138679-40-0 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-[(3-fluorophenyl)amino]-1,3,5-triazin-2-yl]-2,4-dihydro-4-phenyl- (9CI) (CA INDEX NAME)



RN 138679-41-1 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-[4-amino-6-[[2-(methylthio)phenyl]amino]-1,3,5-triazin-2-yl]-2,4-dihydro-4-phenyl- (9CI) (CA INDEX NAME)

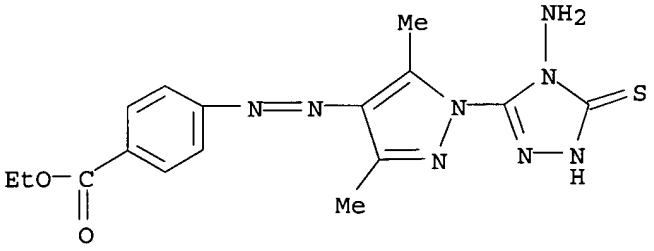


L22 ANSWER 24 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:247213 HCAPLUS
DOCUMENT NUMBER: 114:247213
TITLE: Synthesis and spectrometric analysis of some new azopyrazole substituted 1,2,4-triazole-5-thiones
AUTHOR(S): Rollas, Sevim; Dogan, Nese; Ulgen, Mert; Ozger, Yasemin
CORPORATE SOURCE: Eczacihk Fak., Maramara Univ., Istanbul, Turk.
SOURCE: Marmara Universitesi Eczacilik Dergisi (**1990**), 6(1), 41-7
CODEN: MUEDEZ; ISSN: 1011-3398
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

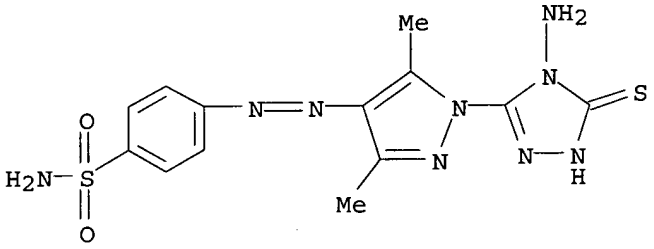


I

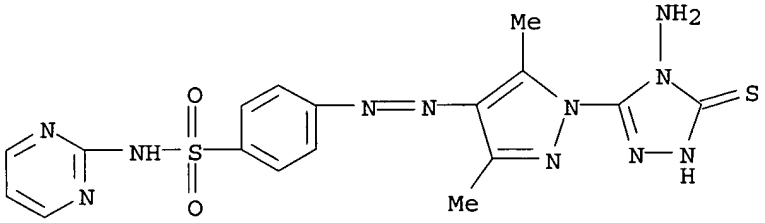
AB Title triazolethione I (R = H, NO2, CO2H, CO2Et, SO2NR1, R1 = H, 4-methyl-2-pyrimidinyl, 4,6-dimethyl-2-pyrimidinyl) were prepared in 51-91%



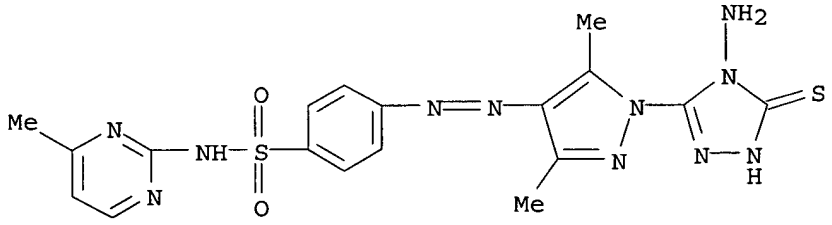
RN 133957-92-3 HCAPLUS
CN Benzenesulfonamide, 4-[[1-(4-amino-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3,5-dimethyl-1H-pyrazol-4-yl]azo]- (9CI) (CA INDEX NAME)

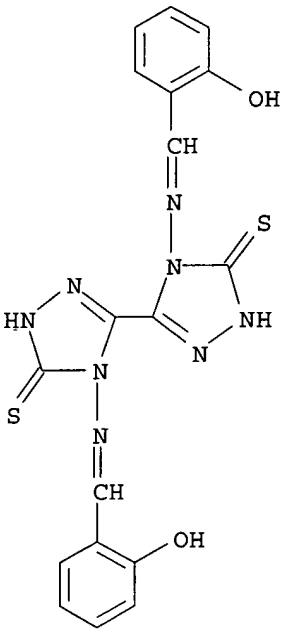


RN 133957-93-4 HCAPLUS
CN Benzenesulfonamide, 4-[[1-(4-amino-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3,5-dimethyl-1H-pyrazol-4-yl]azo]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

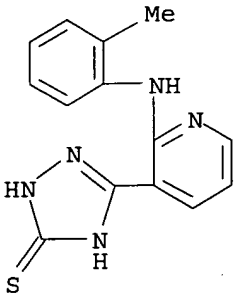


RN 133957-94-5 HCAPLUS
CN Benzenesulfonamide, 4-[[1-(4-amino-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-3,5-dimethyl-1H-pyrazol-4-yl]azo]-N-(4-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

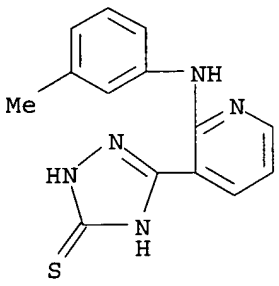




L22 ANSWER 26 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:192613 HCAPLUS
DOCUMENT NUMBER: 110:192613
TITLE: Some novel 2-substituted amino-3-heteroaryl-pyridines as potential antimicrobial agents
AUTHOR(S): Abdel-Gawad, Mona; El-Telbany, F. A.; Badran, Mohga; Ghoneim, Khadiga M.
CORPORATE SOURCE: Fac. Pharm., Cairo Univ., Cairo, Egypt
SOURCE: Egyptian Journal of Pharmaceutical Sciences ( **1988**), 29(1-4), 233-41
CODEN: EJPSBZ; ISSN: 0301-5068
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:192613
GI



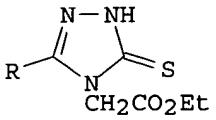
RN 120137-36-2 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 1,2-dihydro-5-[2-[(3-methylphenyl)amino]-3-pyridinyl]- (9CI) (CA INDEX NAME)



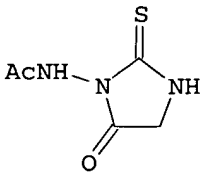
L22 ANSWER 27 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:6027 HCAPLUS
DOCUMENT NUMBER: 108:6027
TITLE: Preparation of alkyl 5-substituted-3-mercapto-4H-1,2,4-triazol-4-yl acetates as antiinflammatories and antibiotic intermediates
INVENTOR(S): Veverka, Miroslav; Marchalin, Miroslav
PATENT ASSIGNEE(S): Czech.
SOURCE: Czech., 5 pp.
CODEN: CZXXA9
DOCUMENT TYPE: Patent
LANGUAGE: Slovak
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| CS 234892 | B1 | 19850416 | CS 1984-882 | 19840207 <-- |
| PRIORITY APPLN. INFO.: | | | CS 1984-882 | 19840207 |

OTHER SOURCE(S): CASREACT 108:6027
GI



I



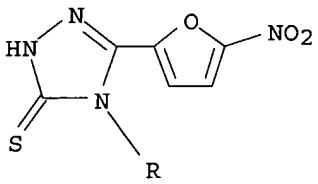
II

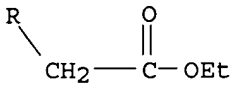
AB Et (3-substituted 5-thioxo-1,2,4-triazolin-4-yl)acetates I (R = e.g. H, Me, Ph, PhCH2, 2-thienyl) were prepared by addition-cyclization reaction of Et isothiocyanatoacetate with carboxylic acid hydrazides in the presence of NaOEt. Thermal cyclization of the adduct AcNHNHCSNHCH2CO2Et in DMF afforded 1-acetamido-2-thiohydantoin II. The effect of substituents on the cyclization course and the thione-thiol tautomerism are discussed.

IT **110167-69-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 110167-69-6 HCAPLUS

CN 4H-1,2,4-Triazole-4-acetic acid, 1,5-dihydro-3-(5-nitro-2-furanyl)-5-thioxo-, ethyl ester (9CI) (CA INDEX NAME)





L22 ANSWER 29 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:608833 HCAPLUS

DOCUMENT NUMBER: 105:208833

TITLE: Oxidation of aldehyde semicarbazones with lead dioxide: application to the syntheses of 2-amino-1,3,4-oxadiazoles and 2,4-dihydro-1,2,4-triazol-3-ones

AUTHOR(S): Thu Huong Nguyen; Milcent, Rene; Barbier, Geo

CORPORATE SOURCE: Fac. Med., Univ. Paris, Paris, 75018, Fr.

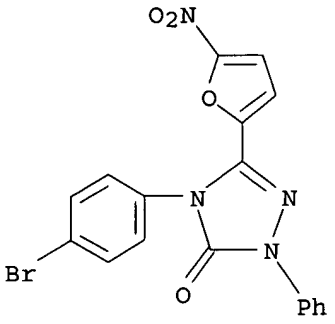
SOURCE: Journal of Heterocyclic Chemistry (**1985**), 22(5), 1383-8
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

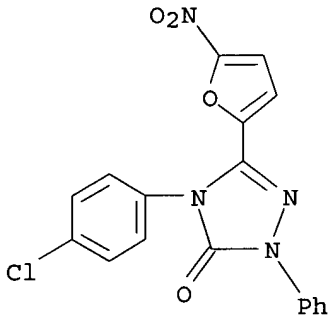
LANGUAGE: English

OTHER SOURCE(S): CASREACT 105:208833

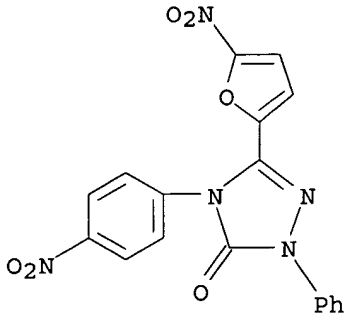
GI



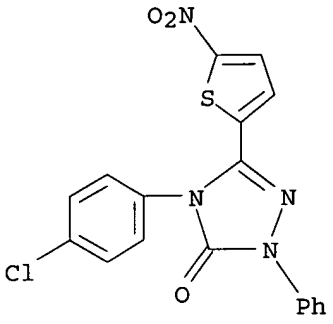
RN 104707-70-2 HCAPLUS
CN 3H-1,2,4-Triazol-3-one, 4-(4-chlorophenyl)-2,4-dihydro-5-(5-nitro-2-furanyl)-2-phenyl- (9CI) (CA INDEX NAME)



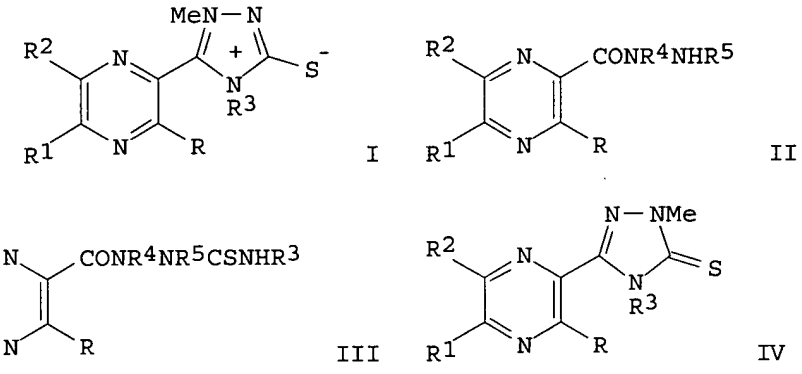
RN 104707-71-3 HCAPLUS
CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-5-(5-nitro-2-furanyl)-4-(4-nitrophenyl)-2-phenyl- (9CI) (CA INDEX NAME)



RN 104707-72-4 HCAPLUS
CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-5-(5-nitro-2-thienyl)-2,4-diphenyl- (9CI) (CA INDEX NAME)

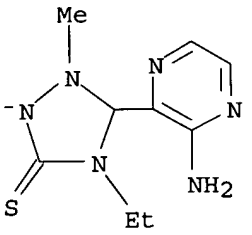


L22 ANSWER 30 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:68940 HCAPLUS
DOCUMENT NUMBER: 96:68940
TITLE: Synthesis of anhydro-3-mercapto-5-pyrazinyl-1,2,4-triazolium hydroxides
AUTHOR(S): Shutske, Gregory M.
CORPORATE SOURCE: Chem. Res. Dep., Hoechst-Roussel Pharm. Inc., Somerville, NJ, 08876, USA
SOURCE: Journal of Heterocyclic Chemistry (**1981**), 18(5), 1017-23
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 96:68940
GI

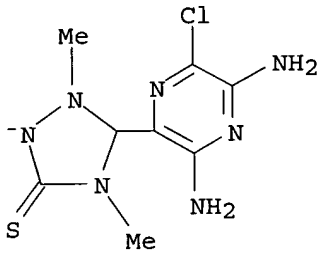


AB The synthesis of some novel anhydro-3-mercapto-5-pyrazinyl-1,2,4-triazolium hydroxides (I; R = H, NH2, NHAc; R1 = H, NH2; R2 = Et, H, Cl; R3 = alkyl, aryl, etc.) is described. The appropriate 1-methylhydrazides II (R4 = Me, R5 = H) were condensed with R3NCS to give the thiosemicarbazides III which were cyclized to I under mildly basic conditions. A few 1,2,4-triazole-3-thiones IV were synthesized for comparison, starting with the 2-methylhdrazides (II; R4 = H, R5 = Me) and then carrying out analogous synthetic transformations.

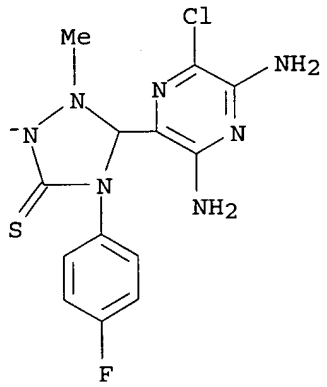
IT **79998-06-4P 79998-07-5P 79998-08-6P**
**79998-09-7P 79998-10-0P 79998-14-4P**
**79998-15-5P 79998-18-8P 79998-19-9P**
**79998-20-2P 80364-55-2P 80364-56-3P**



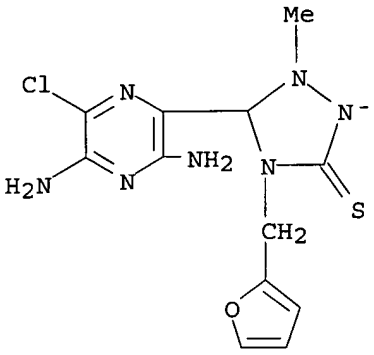
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 79998-10-0 HCAPLUS
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4,5-dihydro-2,4-dimethyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



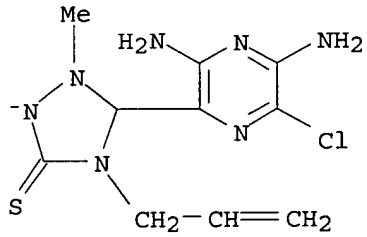
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 79998-14-4 HCAPLUS
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4-(4-fluorophenyl)-4,5-dihydro-1-methyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



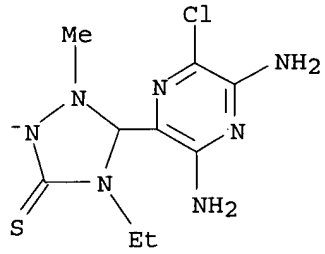
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 79998-15-5 HCAPLUS
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4,5-dihydro-2-methyl-4-phenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 80364-56-3 HCAPLUS
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4,5-dihydro-2-methyl-4-(2-propenyl)-5-thioxo-, inner salt (9CI) (CA INDEX NAME)

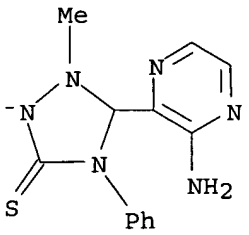


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 80377-35-1 HCAPLUS
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4-ethyl-4,5-dihydro-2-methyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)

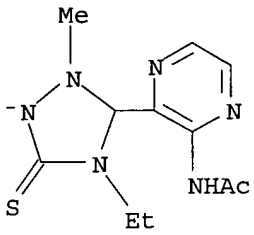


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

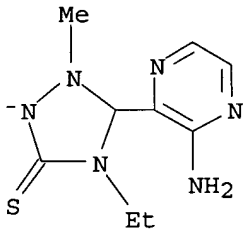
L22 ANSWER 31 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1981:619467 HCAPLUS
DOCUMENT NUMBER: 95:219467
TITLE: 13C-NMR spectra of anhydro-3-mercapto-5-pyrazinyl-1,2,4-triazolium hydroxides
AUTHOR(S): Shutske, Gregory M.; Agnew, Marc N.
CORPORATE SOURCE: Chem. Res. Dep., Hoechst-Roussel Pharm. Inc.,



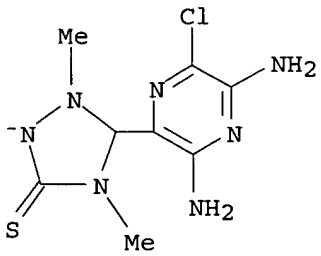
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 79998-08-6 HCAPLUS
CN 1H-1,2,4-Triazolium, 3-[3-(acetylamino)pyrazinyl]-4-ethyl-4,5-dihydro-2-methyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)

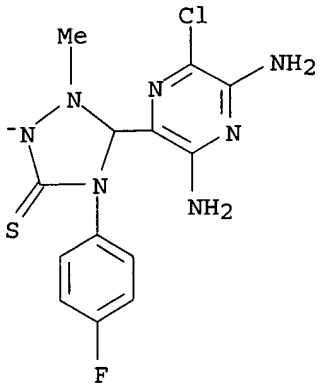


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 79998-09-7 HCAPLUS
CN 1H-1,2,4-Triazolium, 3-(3-aminopyrazinyl)-4-ethyl-4,5-dihydro-2-methyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)

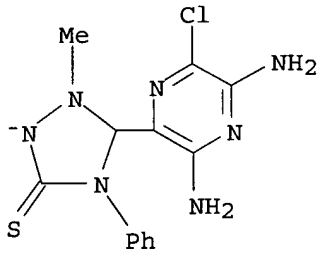


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 79998-10-0 HCAPLUS
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4,5-dihydro-2,4-dimethyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)

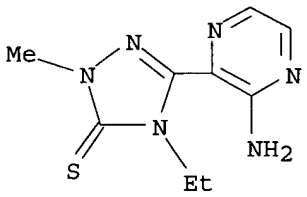




ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 79998-15-5 HCAPLUS
CN 1H-1,2,4-Triazolium, 3-(3,5-diamino-6-chloropyrazinyl)-4,5-dihydro-2-methyl-4-phenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 79998-18-8 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(3-aminopyrazinyl)-4-ethyl-2,4-dihydro-2-methyl- (9CI) (CA INDEX NAME)

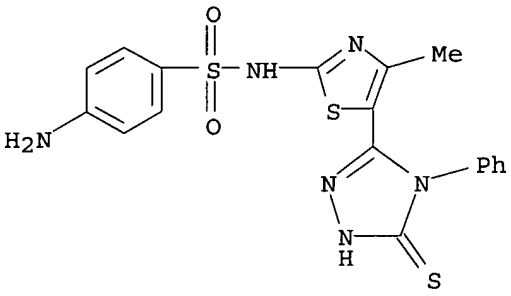


RN 79998-19-9 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(3-aminopyrazinyl)-2,4-dihydro-2-methyl-4-phenyl- (9CI) (CA INDEX NAME)

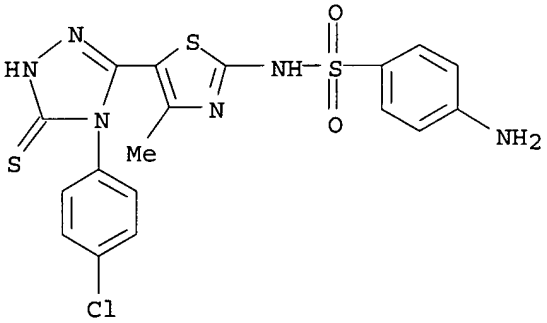
(X = O, S) resp. II (R = 4-ClC6H4) showed fungicidal activity at 200 ppm.

IT **78634-02-3P 78634-06-7P 78634-07-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and fungicidal activity of)

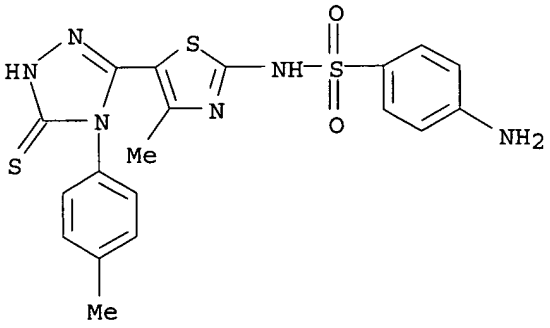
RN 78634-02-3 HCAPLUS
CN Benzenesulfonamide, 4-amino-N-[5-(4,5-dihydro-4-phenyl-5-thioxo-1H-1,2,4-triazol-3-yl)-4-methyl-2-thiazolyl]- (9CI) (CA INDEX NAME)



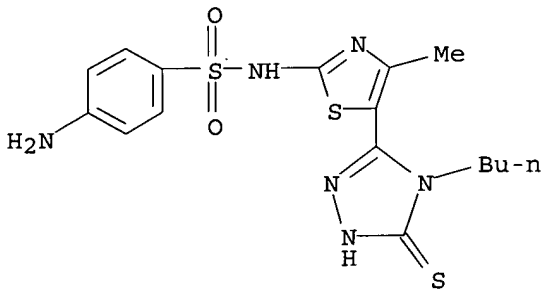
RN 78634-06-7 HCAPLUS
CN Benzenesulfonamide, 4-amino-N-[5-[4-(4-chlorophenyl)-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl]-4-methyl-2-thiazolyl]- (9CI) (CA INDEX NAME)



RN 78634-07-8 HCAPLUS
CN Benzenesulfonamide, 4-amino-N-[5-[4,5-dihydro-4-(4-methoxyphenyl)-5-thioxo-1H-1,2,4-triazol-3-yl]-4-methyl-2-thiazolyl]- (9CI) (CA INDEX NAME)



RN 78634-08-9 HCAPLUS
CN Benzenesulfonamide, 4-amino-N-[5-(4-butyl-4,5-dihydro-5-thioxo-1H-1,2,4-triazol-3-yl)-4-methyl-2-thiazolyl]- (9CI) (CA INDEX NAME)



L22 ANSWER 33 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1979:540850 HCAPLUS
DOCUMENT NUMBER: 91:140850
TITLE: 1-(3-Mercapto-4-substituted-1,2,4-triazol-5-yl)-4-substituted-3-thiosemicarbazides
INVENTOR(S): Eberhardt, Udo; Depner, Johannes; Stopsack, Heinz; Oettel, Michael; Huebler, Doris; Chemnitius, Klaus Henning
PATENT ASSIGNEE(S): Ger. Dem. Rep.
SOURCE: Ger. (East), 20 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

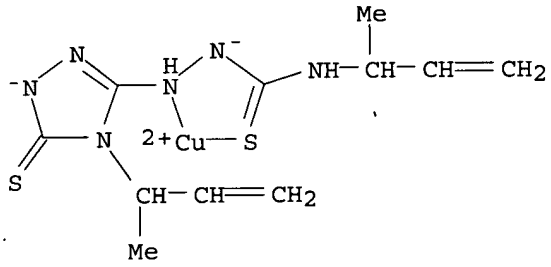
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DD 133436 | Z | 19790103 | DD 1977-201692 | 19771026 <-- |
| PRIORITY APPLN. INFO.: | | | DD 1977-201692 A1 | 19771026 |

GI

RN 71003-46-8 HCAPLUS
CN Copper, [2-[4,5-dihydro-4-(1-methyl-2-propenyl)-5-thioxo-1H-1,2,4-triazol-3-yl]-N-(1-methyl-2-propenyl)hydrazinecarbothioamidato(2-)]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

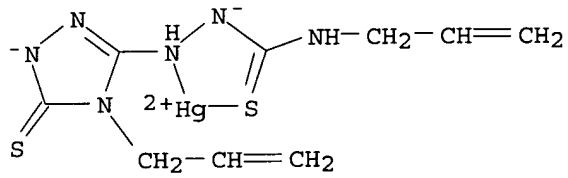
CRN 71003-45-7
CMF C11 H16 Cu N6 S2
CCI CCS



RN 71035-18-2 HCAPLUS
CN Mercury, [2-[4,5-dihydro-4-(2-propenyl)-5-thioxo-1H-1,2,4-triazol-3-yl]-N-2-propenylhydrazinecarbothioamidato(2-)]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

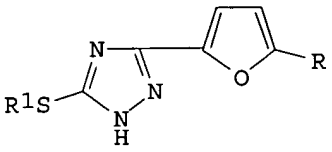
CRN 71035-17-1
CMF C9 H12 Hg N6 S2
CCI CCS



L22 ANSWER 34 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:502330 HCAPLUS
DOCUMENT NUMBER: 87:102330
TITLE: Substituted 5-nitroimidazoles
INVENTOR(S): Asato, Goro; Berkelhammer, Gerald; Gastrock, William Henry
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: U.S., 11 pp. Division of U.S. 3,940,411.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|

DOCUMENT TYPE: Conference
LANGUAGE: Russian
GI



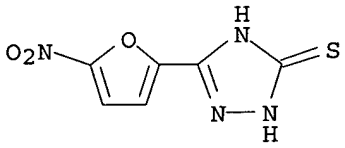
I

AB Nitration of I (R = R1 = H) (II) with HNO3-Ac2O gave I (R = NO2, R1 = H). Treatment of II with furfuryl chloride gave I (R = H, R1 = furfuryl) which was nitrated to give I (R = NO2, R1 = nitrofurfuryl).

IT **57672-16-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with furfuryl chloride)

RN 57672-16-9 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 1,2-dihydro-5-(5-nitro-2-furanyl)- (9CI) (CA INDEX NAME)



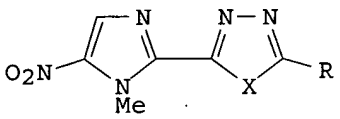
L22 ANSWER 36 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:29722 HCAPLUS
DOCUMENT NUMBER: 86:29722
TITLE: Nitrofuranyl heterocycles. XIII. N-Methyl-3-methylthio-5-(5-nitro-2-furanyl)-1H-1,2,4-triazoles
AUTHOR(S): Benjamin, Louis E.; Snyder, Harry R., Jr.
CORPORATE SOURCE: Norwich Pharmacal Co. Div., Morton-Norwich Prod., Inc., Norwich, NY, USA
SOURCE: Journal of Heterocyclic Chemistry (**1976**), 13(5), 1115-18
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

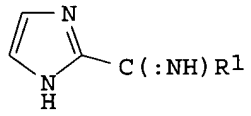
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 3940411 | A | 19760224 | US 1973-409505 | 19731025 <-- |
| US 3649638 | A | 19720314 | US 1969-863378 | 19691002 <-- |
| AT 292692 | B | 19710910 | AT 1969-9579 | 19691010 <-- |
| FR 2020451 | A5 | 19700710 | FR 1969-35003 | 19691013 <-- |
| FR 2020451 | B1 | 19740111 | | |
| US 3790589 | A | 19740205 | US 1971-202568 | 19711126 <-- |
| US 4026903 | A | 19770531 | US 1975-632941 | 19751118 <-- |

PRIORITY APPLN. INFO.: US 1968-766984 A2 19681011
US 1969-863378 A3 19691002
US 1971-202568 A3 19711126
US 1973-409505 A3 19731025

GI


I

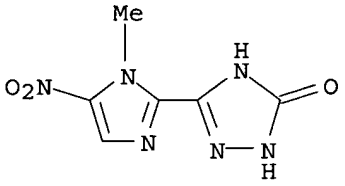

II

AB The imidazoles I (R = Me, H2N, X = NH; R = H2N, X = O, S) were prepared Thus, II (R1 = EtO) was treated with MeCONHNH2 to give II (R = MeCONHNH), which was cyclized with HOAc to give I (R = Me, X = NH) (III). At 160 mg/kg I (R = H2N, X = S) cured pullet chicks infected with Escherichia coli. At 200 mg/kg III cleared mice infected with Trichomonas vaginalis.

IT **27344-17-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 27344-17-8 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 1,2-dihydro-5-(1-methyl-5-nitro-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)



L22 ANSWER 38 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1976:4868 HCAPLUS
DOCUMENT NUMBER: 84:4868
TITLE: 1,2,4-Triazole derivatives
AUTHOR(S): Lipanova, M. D.; Burov, E. V.; Kulikova, L. K.
CORPORATE SOURCE: USSR
SOURCE: Issled. V Obl. Sinteza I Kataliza Organ. Soedinenii ( **1975**) 29
From: Ref. Zh., Khim. 1975, Abstr. No. 16ZH259
DOCUMENT TYPE: Journal

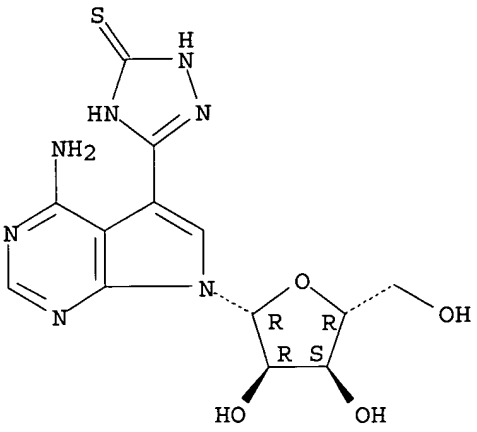
group which can be accommodated at C5 without a complete loss of activity. All of the 5-membered heterocyclic rings showed some activity. Activity was highest when the ring was nonarom. and a 5-membered nonarom. ring was more active than a 6-membered nonarom. ring. None of these derivs. were as active as the compds. with smaller nonannulated groups at position 5.

IT **55470-38-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and neoplasm inhibiting activity of)

RN 55470-38-7 HCAPLUS

CN 3H-1,2,4-Triazole-3-thione, 5-(4-amino-7-β-D-ribofuranosyl-7H-pyrrolo[2,3-d]pyrimidin-5-yl)-1,2-dihydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




L22 ANSWER 40 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1974:563330 HCAPLUS

DOCUMENT NUMBER: 81:163330

TITLE: Nitrofurans with high renal excretion

AUTHOR(S): Akerblom, Eva B.

CORPORATE SOURCE: Dep. Org. Chem., Pharm. AB, Uppsala, Swed.

SOURCE: Journal of Medicinal Chemistry (**1974**), 17(7), 756-8
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

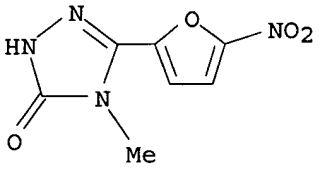
AB Of the 16 title compds. tested, those with acidic groups were prepared by reaction of Et haloacetate with the Na salt of the appropriate nitrofuran compound, while those with the nitroamino group were prepared by nitration of the corresponding amino compds. The in vitro antibacterial activity of the new compds. was low, with the esters showing more activity than the acids. Against Trichomonas vaginalis, the esters I [52980-64-0] and II [27550-27-2] show very high activity. II [**52980-53-7**] and IV [52980-65-1], tested for peroral absorption and urinary excretion in dogs, were >60% recovered in the urine. Urinary excretion was blocked by probenicid, indicating tubular excretion.

IT **52980-62-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of)

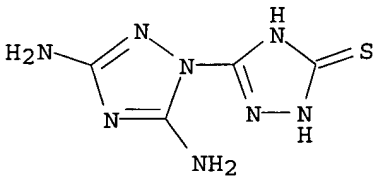
RN 52980-62-8 HCAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-methyl-5-(5-nitro-2-furanyl)-,

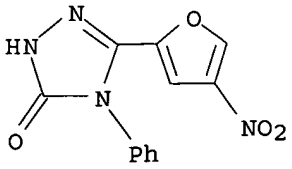
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and bactericidal activity of)
RN 41735-59-5 HCAPLUS
CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-methyl-5-(5-nitro-2-furanyl)- (9CI) (CA INDEX NAME)



L22 ANSWER 42 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1972:564610 HCAPLUS
DOCUMENT NUMBER: 77:164610
TITLE: Reactions of 3-hydrazino-1,2,4-triazoles with dicyandiamide
AUTHOR(S): Uteg, Karl Heinz
CORPORATE SOURCE: Bezirksinst. Blutspende- Transfusionswes., Schwerin, Ger. Dem. Rep.
SOURCE: Zeitschrift fuer Chemie (**1972**), 12(8), 291
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Refluxing the triazoles (I, R = H, SH, Ph, o-ClC6H4, o-MeOC6H4, o-, m-, p-MeC6H4) with H2NC(:NH)NHCN in HCl-H2O yielded 36-68 guanazoles (II). Uv spectroscopic data of II were reported.
IT **38767-47-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38767-47-4 HCAPLUS
CN 3H-1,2,4-Triazole-3-thione, 5-(3,5-diamino-1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)



L22 ANSWER 43 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1972:526568 HCAPLUS
DOCUMENT NUMBER: 77:126568
TITLE: Synthesis of pyrazine derivatives as potential hypoglycemic agents
AUTHOR(S): Ambrogi, V.; Bloch, K.; Daturi, S.; Logemann, W.; Parenti, M. A.
CORPORATE SOURCE: Antidiabetic Dep., Carlo Erba Res. Inst., Milan, Italy



L22 ANSWER 45 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1970:425480 HCAPLUS
DOCUMENT NUMBER: 73:25480
TITLE: 1,2-Disubstituted 5-nitroimidazoles
INVENTOR(S): Asato, Goro; Berkelhammer, Gerald; Gastrock, William H.; Starer, Ira; Papaioamiou, Christos G.; Albright, Jay D.; Shepherd, Robert G.
PATENT ASSIGNEE(S): American Cyanamid Co.
SOURCE: Ger. Offen., 44 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

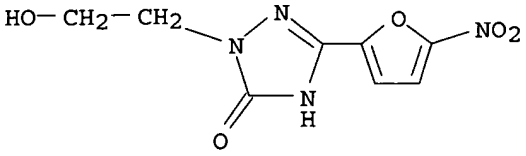
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 1951259 | A | 19700527 | DE 1969-1951259 | 19691010 <-- |
| US 3652555 | A | 19720328 | US 1969-833683 | 19690616 <-- |
| AT 292692 | B | 19710910 | AT 1969-9579 | 19691010 <-- |
| FR 2020451 | A5 | 19700710 | FR 1969-35003 | 19691013 <-- |
| FR 2020451 | B1 | 19740111 | | |

PRIORITY APPLN. INFO.: US 1968-766984 A 19681011
US 1969-833683 A 19690616

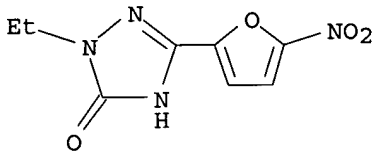
GI For diagram(s), see printed CA Issue.

AB The title compds. (I and II), active against chicken typhus, enteritis, colibacillosis, and Trichomonas vaginalis, were prepared I (X = NH) were prepared by treatment of the corresponding Et 5-nitroimidazole-2-carboximidates, obtained from 5-nitro-2-cyanoimidazoles (III), with acylhydrazines, H2NNHC(:NH)NH2, H2NNHCONH2, or H2NNHCSNH2. Reaction of the corresponding 5-nitro-2-(chloroformyl)imidazoles with H2NNHCONH2 or H2NNHCSNH2 gave I (X = O). The following I were prepared (R, R1, and X given): Me, Ac, NH (Ia); Me, C(:NH)NH2, NH; Me, CONH2, NH; Me, CSNH2, NH; Me, CSNH2, O; HOCH2CH2, CSNH2, O; Me, CONH2, O; AcOCH2CH2, CSNH2, NH; and BzOCH2CH2, CSNH2, NH. Cyclization of I gave the following II (R, R2, and Y given): Me, Me, NH; Me, NH2, NH; Me, NH2, S (IIa); Me, NH2, O; BzOCH2CH2, NH2, S; and HOCH2CH2, NH2, S. II (Y = S) were also directly obtained from III by treating III with H2NNHCSNH2 in the absence of H2O and in the presence of a strong acid. Chickens, infected with chicken typhus, were treated with food containing 0.1% Ia or 0.05% IIa. Of 5 chickens all survived, whereas of 20 untreated chickens all died.

IT **27344-17-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 27344-17-8 HCAPLUS
CN 3H-1,2,4-Triazol-3-one, 1,2-dihydro-5-(1-methyl-5-nitro-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)



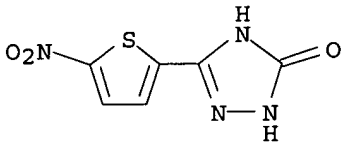
RN 25142-90-9 HCAPLUS
CN 3H-1,2,4-Triazol-3-one, 2-ethyl-2,4-dihydro-5-(5-nitro-2-furanyl)- (9CI) (CA INDEX NAME)



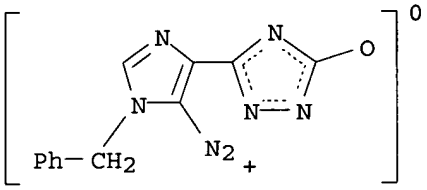
L22 ANSWER 47 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:106436 HCAPLUS
DOCUMENT NUMBER: 70:106436
TITLE: Heteroaromaticity. XX. Novel thermal 1,3-dipolar cycloaddition of 5-nitrofuran-2-carbohydroxamoyl chloride with diketene and dicyclohexylcarbodiimide
AUTHOR(S): Sasaki, Tadashi; Yoshioka, Toshiyuki
CORPORATE SOURCE: Nagoya Univ., Nagoya, Japan
SOURCE: Bulletin of the Chemical Society of Japan (**1969**), 42(1), 258-60
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 5-Nitrofuran-2-carbohydroxamoyl chloride (I) was heated in toluene with diketene until the evolution of HCl stopped. Spectral data and elemental anal. confirmed that the product was 3-(5-nitro-2-furyl)-5-methylisoxazole, m. 143-4°. I was heated in toluene with an equivalent amount of dicyclohexylcarbodiimide (II) until the evolution of HCl ceased. After removal of the solvent under reduced pressure, the residue was dissolved in CHCl3 and chromatographed on a silica gel column to give 1,4-dicyclohexyl-3-(5-nitro-2-furyl)-4,5-dihydro-5-oxo-1H-triazole (III). When an ethanolic solution of III was refluxed with EtONa, 1,3-dicyclohexylurea was recovered. Thermal treatment of 5-nitrofuran-2-carboxaldehyde oxime with II and the normal treatment of 5-nitrofuran-2-carbonitrile oxide with II in ether at room temperature both gave 5-nitrofuran-2-carbonitrile and no cyclization occurred. Possible reaction mechanisms were discussed.

IT **22200-72-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 22200-72-2 HCAPLUS
CN Δ2-1,2,4-Triazolin-5-one, 1,4-dicyclohexyl-3-(5-nitro-2-furyl)- (8CI) (CA INDEX NAME)



L22 ANSWER 49 OF 50 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1967:443155 HCAPLUS
DOCUMENT NUMBER: 67:43155
TITLE: Diazo-β-azomethine-v-triazine equilibrium
AUTHOR(S): Temple, Carroll, Jr.; Kussner, Conrad L.; Montgomery, John A.
CORPORATE SOURCE: Kettering-Meyer Lab., Southern Res. Inst., Birmingham, AL, USA
SOURCE: Journal of Organic Chemistry (**1967**), 32(7), 2241-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The nitrosation of some 3-[5- (or 4-)aminoimidazol-4-(or 5-)-yl]-s-triazoles and 5-[5- (or 4-)-aminoimidazole-4- (or 5-)-yl]tetrazoles is described. The resulting diazoimidazole-v-triazine systems are used to study the effect of solvent and certain groups on the diazo-β-azomethine-v-triazine equilibrium Structure assignments are based on data obtained from the ir and proton N.M.R. spectra. 10 references.
IT **12129-55-4P 13976-26-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 12129-55-4 HCAPLUS
CN Imidazole-5-diazonium, 1-benzyl-4-(5-hydroxy-s-triazol-3-yl)-, hydroxide, inner salt (8CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 13976-26-6 HCAPLUS
CN s-Triazol-3-ol, 5-(5-amino-1-benzylimidazol-4-yl)-, monohydrochloride (8CI) (CA INDEX NAME)

AB New substituted nitrofuryltriazolines, I, where R can be H, Me, Ac, CH2CH2OH, or diethoxythiophosphoryl, and R1 can be O, imino (substituted or not), or acetylimino, are used as antiseptics and antiparasitics. Dry HCl is passed through a cooled mixture of 900 g. 5-nitro-2-furonitrile and 5450 cc. anhydrous EtOH for 3.5-4.5 hrs. The solid is filtered off, washed with 150 cc. EtOH, and anhydrous Et2O to give 808 g. ethyl 5-nitro-2-furimidate-HCl (II), m. 158-60°. A mixture of 100 g. II, 84 g. semicarbazide, and 300 cc. EtOH is heated at 50-5° 30 min. with stirring, cooled, and diluted with 2000 cc. water. The product is filtered off to give 60 g. 5-nitro-2-furamidine-N-ureide (III), m. 274-5°. A solution of 60 g. III in 450 cc. nitrobenzene is refluxed 15 min., cooled, and diluted with 400 cc. Et2O. The solid is filtered off, washed with Et2O, and crystallized (water) to give 31 g. 5-oxo-3-(5-nitro-2-furyl)-Δ2-1,2,4-triazoline, m. 277-9°. II (110 g.) is added to a solution of 55 g. aminoguanidine-HCl in 600 cc. HCONMe2. The solution is heated at 50-60° 30 min., cooled, and diluted with Et2O. The oily solid is washed with EtOH and Et2O, and dried to give 90 g. 5-nitro-2-furamidine-N-guanidine-2HCl (IV), m. 204-5°. A solution of 90 g. IV in 400 cc. nitrobenzene is refluxed 15 min., filtered, cooled, and diluted with Et2O. The solid is filtered off, washed with Et2O and dried to give 32 g. 5-imino-3-(5-nitro-2-furyl)-Δ2-1,2,4-triazoline (V), m. 289-90° (H2O). A mixture of 110 g. II, 45 g. 2-methylsemicarbazide, and 500 cc. EtOH is heated at 50-60° 1 hr., cooled, and diluted with Et2O. The solid is filtered off to give 100 g. 5-nitro-2-furamidine-N-(1-methylureide)-HCl (VI), which is treated with Na2CO3 to give 5-nitro-2-furamidine-N-(1-methylureide), m. 185-6°. A solution of 100 g. VI in 400 cc. nitrobenzene is refluxed 15 min., cooled, and diluted with Et2O. The solid is filtered off, and washed with Et2O, to give 35 g. 1-methyl-5-oxo-3-(5-nitro-2-furyl)-Δ2-1,2,4-triazoline, m. 275-6° (H2O). A mixture of 20 g. V, 10 cc. Ac2O, and 300 cc. anhydrous AcOH is heated on a water bath for 20 min., cooled, and diluted with Et2O. The solid is filtered off and crystallized (HCONMe2-water) to give 30 g. 1-acetyl-5-imino-3-(5-nitro-2-furyl)-Δ2-1,2,4-triazoline (VII). Dry HCl (5.5 g.) is introduced into a solution of 29 g. V in 580 cc. anhydrous AcOH. The solution is heated 20 hrs., cooled, and diluted with water. The solid is filtered off to give 25 g. 5-acetylimino-3-(5-nitro-2-furyl)-Δ2-1,2,4-triazoline (VIII), m. 343-5° (HCONMe2). VII (4.8 g.) is added with stirring to 20 g. benzophenone at 290°. The mixture is heated at 290-5° 2 min., cooled, and diluted with Et2O, and the solid filtered off to give VIII, m. 343-5° (HCONMe2). A mixture of 24 g. II, 24 g. 2-(2-hydroxyethyl)semicarbazide, and 300 cc. EtOH is heated at 50-60° 30 min., cooled, and diluted with Et2O. The solid is filtered off, and dissolved in water. This solution is filtered, alkalized with Na2CO3, cooled, and the solid filtered off to give 20 g. 5-nitro-2-furamidine-N-[1-(2-hydroxyethyl)ureide], m. 175-80°, which treated with dry HCl in a suitable solvent gives 5-nitro-2-furamidine-N-[1-(2-hydroxyethyl)ureide]-HCl (IX). A mixture of 144 g. IX and 400 cc. nitrobenzene is refluxed 15 min., filtered, cooled, and diluted with Et2O. The solid is filtered off and washed with 50% AcOH to give 45 g. 1-(2-hydroxyethyl)-5-oxo-3-(5-nitro-2-furyl)-Δ2-1,2,4-triazoline, m. 263-4° (AcOH). A mixture of 58.5 g. V, 56.7 g. diethylthionophosphoryl chloride, 16.2 g. NaOMe, and 1200 cc. EtOH is refluxed 30 min., filtered, cooled, and diluted with water. The solid is filtered off to give 29 g. 1-(O,O-diethyl thiophosphate)-5-imino-3-(5-nitro-2-furyl)-Δ2-1,2,4-triazoline, m. 160-1° (MeOH). A solution of 37.2 g. 1-amino-1-methylguanidine-HCl, and 66.3 g. II in 300 cc. HCONMe2 is heated at 50-60° 30 min., cooled, and diluted with Et2O. The gummy precipitate is washed with Et2O, and dried to give 5-nitro-2-furamidine-

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